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The imported fire ants, *Solenopsis invicta*, were introduced into the United States by way of Alabama in the mid 1930s. Their devastating impact on the agriculture of the south led to a project to eradicate them, which in turn resulted in the discovery of the antiangiogenic activity of a component of their venom. The discovery of 2-methyl-6-alkyl piperidines has led to the synthesis and study of solenopsin A, a *trans*-2-methyl-6-*n*-undecyl piperidine and analogs. Solenopsin A has proven effective in biological testing of zebrafish for antiangiogenic studies, thus qualifying it and its analogs as viable candidates for further studies.

Angiogenesis, a term coined by P. Shubik in 1968, is the growth of blood vessels from previously existing vessels. Angiogenesis is a normal physiological process in humans during early childhood development, but seldom in adults. The dominant disease that is affected by angiogenesis is cancer, which progresses through tumor growth. Angiogenesis inhibition, also termed antiangiogenesis, appears to have a very exciting future in cancer therapy. Antiangiogenic molecules have been prepared and studied as potential new therapeutics, and they should be advantageous over the commonly used cancer therapies. Several Williamson ether techniques were investigated to develop analogs of solenopsin A to submit for biological testing as antiangiogenic agents.

Computational chemistry techniques were utilized to gain insight into conformation preferences for the ether products. Each molecule was calculated using

quantum and molecular mechanics in Spartan. The calculations were performed using equilibrium geometry and the Hartree-Fock model with the 6-31G* basis set. Each structure was subject to a molecular mechanics conformer search followed by quantum mechanical calculations for the lowest energy conformers. The dihedral angles were recorded for each conformer, and again for the minimized conformers.

SYNTHETIC AND MOLECULAR MODELING STUDIES OF ANTIANGIOGENIC COMPOUNDS BASED ON SOLENOPSIN A LEAD STRUCTURE

by

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APPROVAL PAGE

This thesis has been approved by the following committee of the Faculty of The Graduate School at The University of North Carolina at Greensboro.

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Date of Final Oral Examination

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CHAPTER I

SYNTHETIC STUDIES OF SOLENOPSIN A ANALOGS

Introduction

The imported fire ants, *Solenopsis invicta*, were introduced into the United States by way of Alabama in the mid 1930s. Their devastating impact on the agriculture of the south led to a project to eradicate them, which in turn resulted in the discovery of the antiangiogenic activity of a component of their venom. The discovery of 2-methyl-6-alkyl piperidines has led to the synthesis and study of solenopsin A, *trans*-2-methyl-6-*n*-undecyl piperidine, and analogs. Solenopsin A has proven effective in biological testing of zebrafish for antiangiogenic studies, thus qualifying it and its analogs as viable candidates for further studies.

Background

Angiogenesis, a term coined by P. Shubik in 1968, is the growth of blood vessels from previously existing vessels.[1] Angiogenesis is a normal physiological process in humans during early childhood development, but seldom in adults. It is relatively non-existent in adults except for menstruation, wound healing, and diseases which are dependent on vascularization, such as arthritis and diabetes retinopathy.[2,3] In both arthritis and diabetes, new blood vessels form which destroy cartilage and cause

blindness, respectively. The dominant disease that is coupled with angiogenesis is cancer, which progresses through tumor growth.

The role of angiogenesis inhibitors in arresting tumor growth was first hypothesized by Dr. Judah Folkman in 1971, which was an outgrowth of his observations and G. H. Algire's initial idea of tumor growth and the necessity for blood vessels relevancy in 1947.[4] Since its discovery, angiogenesis has emerged as a serious target for understanding the physiology of tumor progression and metastasis, which are "cancerous cells that have spread to a completely new location".[5] There is an extended amount of time in which the tumor is not affected by angiogenesis. During this time period a tumor is able to maintain a limited size of a few millimeters. Once angiogenic properties are introduced to the tumor, new blood vessels promote tumor growth and ultimately metastasis.[6] There are several important points of Dr. Folkman's prediction of angiogenesis dependence which are essential in understanding the fundamentals for the research and development of potential cancer therapies. These points include the following: the size and activity of a tumor, such as dormancy which is maintained with a limited tumor size; tumor masses "activate" angiogenesis; the angiogenesis switch is triggered by tumor angiogenic factors; tumor growth can be affected by disrupting tumor angiogenesis; and sustained regression of tumor sizes 1-2mm.[1]

With the discovery that "angiogenesis plays an important role in cancer from the initial stage of carcinogenesis to the end stage of metastatic disease", angiogenesis inhibition became an aim in cancer therapy.[6] Angiogenesis inhibition, also termed

antiangiogenesis, appears to have an exciting future in cancer therapy. Antiangiogenic molecules have been prepared and studied as potential new therapeutics, and they should be advantageous over the commonly used cancer therapies. Based on previous research, it has been determined that antiangiogenic techniques are favorable compared to traditional anti-cancer methods due to its non-problematic interaction with drugs and lower toxicity effects.[7] Some suggested guidelines for the development of antiangiogenic compounds include low toxicity, prolonged use, drug resistance, and a combination with cytotoxic therapies.[8] A number of notable advantages include tumor specifity, low toxicity, mainstream of cancer therapy, and continuous dormancy of tumors.[7] There are, however, several limitations along with the advantages of this novel therapeutic method. Antiangiogenic therapies would require long term treatment, leading to an interaction of repair and regression, and the drug interaction with long term therapy may not be as effective as desired.[2] The investigation of antiangiogenic compounds commenced nearly thirty years ago, and the results have yielded both promising and troubling data. The advantages are worthy of notice, but the discovery of its uses also resulted in problems with the clinical investigations. The limitations expressed through clinical studies include lack of rapid transformation of the tumors and the need for combination treatments with cytotoxic drugs.[1] This combination treatment of drugs involves de-bulking and vascularization inhibition, which is achieved with the cytotoxic and antiangiogenic therapies, could result in survivors of the disease.[9]

Long term research has produced an antiangiogenic drug phenomenon, such that this research has become one of the main focuses for cancer therapies. The development of angiogenic inhibitors through laboratory investigations will need to be clinically researched for further promotion to clinical trials. With recent discoveries, inhibitors will be designed with the ideal characteristics in place.

An example of a specific type of cancer that can be positively affected by the use of antiangiogenic therapies is hepatocellular carcinoma (HCC). HCC is one of the five most common cancers. This liver disease is associated with cirrhosis and impaired liver function. The sensitivity and delicacy of the liver makes HCC a very difficult cancer to treat. Conventional therapies currently consist of "surgical resection, liver transplant, locoregional therapies, and standard cytotoxic therapies." Due to the lack of efficacy of conventional therapies, the investigation of antiangiogenic therapies and their success in other cancers may prove helpful in the eradication of hepatocellular carcinoma.[6]

The imported fire ant has played a negative role in the agricultural infrastructure of the southeastern United States. This formidable pest, which has caused incessant havoc to crops, livestock, and humans, possesses a key component in its venom that could potentially cure cancer. The imported fire ant is more formally known as *Solenopsis invicta* which originated in Mato Gross, Brazil. *Solenopsis invicta* was imported into the United States via Mobile, Alabama between 1933 and 1945. They now occupy states ranging from the Carolinas to Texas. The limited spread northward is due to the severe winters which destroy *S. invicta's* chances of survival because of their inability to

hibernate. Similary, limited spread to the west is due presumably to the harsh desert climate in Texas.[10]

The imported fire ant's presence in the United States has caused a number of serious problems which include "feeding on plants, stinging of livestock, damage to farm machinery that strike mounds, loss of hay and grazing area, refusal of workers to enter heavily infested fields to cultivate or harvest crops, and hazards to human health from stings that may cause systemic reaction or complications from secondary infections".[10] Although there are a number of problems associated with fire ants, more specifically the cause of most problems is the use of their potent venom as a defense mechanism. The venom released from stings may result in allergic reactions such as vomiting, dizziness, perspiration, and asthma. In severe cases, if medical assistance is not received, the individual may die. Although painful and potentially deadly, the venom possesses insecticidal, bactericidal, and fungicidal properties. In efforts to rectify or control the problem of *S. invicta*, the venom was investigated and was found to reveal 2-methyl-6-alkyl piperidines. In the investigation of solenopsin, five components of the venom were isolated and synthesized: solenopsin A (trans-2-methyl-6-*n*-undecylpiperidine),**1**, B (trans-2-methyl-6-*n*-tridecylpiperidine),**2**, and C (trans-2-methyl-6-*n*-pentadecylpiperidine),**3**, as well as dehydrosolenopsin B (trans-2-methyl-6(*cis*-4-tridecenyl)piperidine,**4**, and C (trans-2-methyl-6(*cis*-6-pentadecenyl)piperidine,**5** (Figure 1).[10]

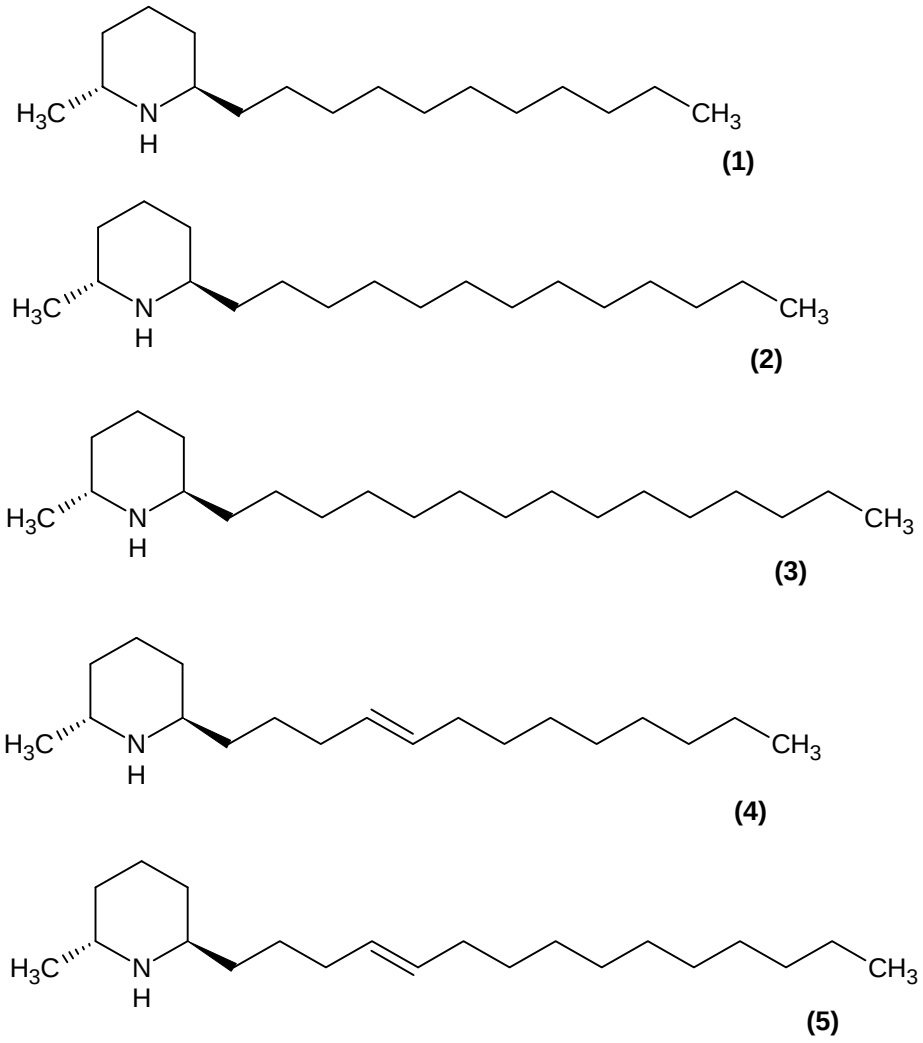


Figure 1: Solenopsin Venom

The solenopsin venom of *Solenopsis invicta* was investigated through sustained virological response (SVR) angiogenesisis assay to reveal antiangiogenic activity.[11] The assay resulted in inhibition of angiogenesis in zebrafish. Arbiser, Bowen, and collaborators investigated the bioactivity of the solenopsin venom with Akt, a key enzyme in angiongenesis, which is involved in proliferation, cytoskeletal organization,

survival, and malignant transformation. Due to the fact that Akt plays this particular role in angiogenesis makes it a logical anticancer treatment target. In order to properly analyze the potential of solenopsin A, it was necessary to synthesize it and several derivatives. There were several methods reported and used to synthesize the analogs which utilize 4-chloropyridine and alkyl magnesium halides as starting reagents in a subsequent process of N-Boc-piperidine lithiation and methylation, and the procedure of Beak and Lee.[11] The synthesis and testing of solenopsin A and sixteen tetrahydropyridine analogs as antiangiogenic compounds revealed that only solenopsin A made a significant difference in the SVR proliferation.

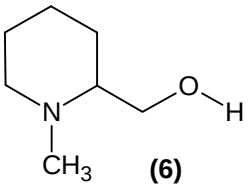
Results and Discussion

Several solenopsin A derivatives were envisioned which maintained the piperidine ring skeleton with variations made only to the side chains. The decision to implement an oxygen moiety in the side chain is several fold: (1) enhanced activity, (2) disrupt potential for micelle formation. The synthetic strategy was to use the Williamson ether synthesis, for preparation of the desired analogs. This approach was chosen based on assumed ease of synthesis. Ideally, the alkoxide would be formed from use of a strong base, such as sodium hydride, and the alkylation of the alkoxide would follow with a simple alkyl halide. The next step would include addition of a long chain carbon to investigate the biological activity that was documented by Arbiser et al[11].

The investigation of solenopsin A derivatives included a thorough search of scientific databases to verify that these substrates have not been previously synthesized

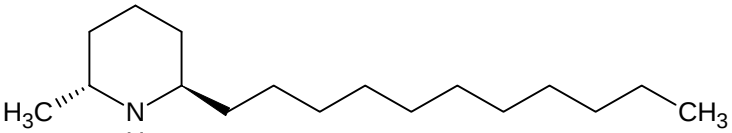
and submitted for antiangiogenic testing. A literature search for comound previously synthesized did not yield direct procedures for our use; however, modifications were made based on availability of substrates and reagents, and laboratory conditions.

The investigation of novel analogs began with (1-methylpiperidin-2-yl)methanol, **6**, (Figure 2). The goal was to alkylate the side chain using the proposed Williamson ether synthesis, while ignoring the group previously occupied by the methyl group in solenopsin A, **1**, (Figure 3).



(6)

Figure 2: N-methyl-2-piperidine methanol

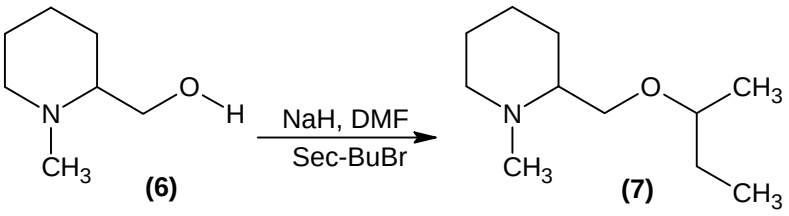


(1)

Figure 3: Solenopsin A

The initial synthesis consisted of the N-methyl-2-piperdine methanol, **6**, and treatment with sec-butyl bromide. Simple proton-NMR identification was used in an attempt to identify the ether product (Scheme 1). The procedure was modified from that of Pan et al.[12] The same substrate was again used to develop the ether using a procedure relayed by Hsiang-Ru Lin et al.[13] The difference in procedures included the use of heat

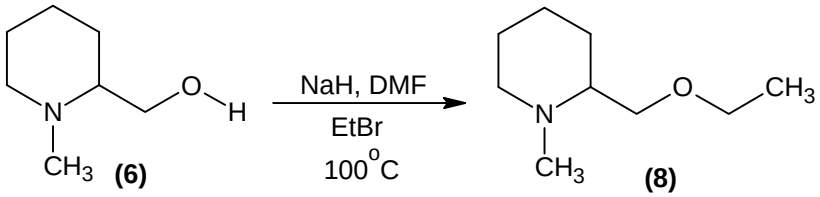
and a longer reaction time. Neither reaction yielded the desired products, even though the TLCs concluded that the reaction was complete. Due to the complexity of the proton NMR, and, in order to calibrate our results, it was decided to use a simpler alkane, ethyl bromide, for the modification of the alcohol. The secondary halide was used due to its ready availability, even though it is ideal to complete a Williamson ether synthesis using a primary halide.



Scheme 1: sec-Bu Ether

Next, was the use of bromoethane as a substrate utilizing the same starting material, **5**. Several reactions were developed and reported using this compound for ether preparation. The first of these was by Sallay et al. in which the ethyl ether was not produced due to the mixture refluxing over night at an extreme temperature and essentially producing a darkened hard mass that did not yield the desired product (Scheme 2).[14] This procedure was repeated again using a lower temperature but the same reaction time. The modification also did not yield the product, although the crude material was an oil instead of a solid substance. With the failure to create the desired material using the method by Pan et al., the bromoethane was again used in the same

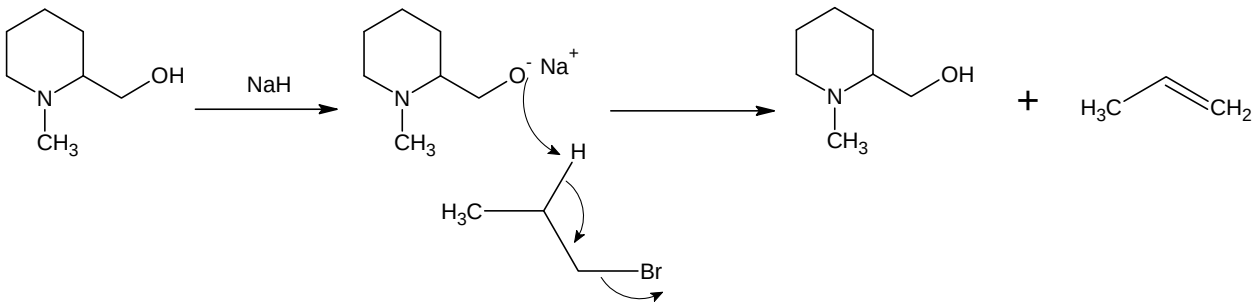
procedure as that of the use of sec-butyl bromide. The procedure used for the second sec-butyl bromide reaction by Hsiang-Ru Lin et al. was used for bromoethane.[13] This again yielded a dark solid substance which is presumably due to the excessive heating for a prolonged overnight reaction time. Unable to produce the desired material led to the investigation of another procedure by Boschelli et al.[15] Medicinal Chemistry suggested methodology involved refluxing the reagents before completing the reaction at room temperature.[15] The alternative method involved refluxing the reagents before completing the reaction at room temperature. Although thin layer chromatography afforded a less polar spot, which is expected, the desired product was still not produced.



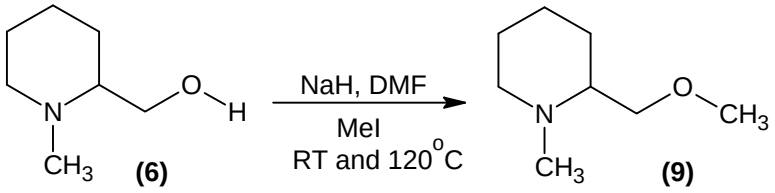
Scheme 2: Ethyl Bromide Ether

In our efforts to further explore the reaction, an eleven carbon chain was then attempted using 11-chloro-1-undecen in the previously stated procedure[15] to assist in the proton identification of the NMR analysis. The TLC again produced a less polar spot, but iodine was also used in an attempt to further identify the presence of possible products that may not be as easily visualized through ultraviolet light or phosphomolybdic acid. The attempted purification yielded no conclusion as to the presence of the desired ether.

With lack of progress in the derivative synthesis, simultaneous reactions were performed again utilizing bromoethane. The simplified reactions consisted of running one at room temperature and the other at approximately 120^{o}C. Still, isolating and identifying the ether product was illusive. The use of methyl iodide became an option in trying to understand the complexity of the reaction and possible inter- and intra-molecular reactions. With the use of iodomethane instead of bromoethane, the possibility of an elimination reaction could be dismissed (Scheme 3). The use of methyl iodide was reacted using the same simplified procedure as that of the bromoethane: simultaneous room temperature and refluxed methods (Scheme 4). This alkyl chain alteration also proved inconclusive in determining the possible molecular properties present with these particular substrates.



Scheme 3: Elimination Reaction



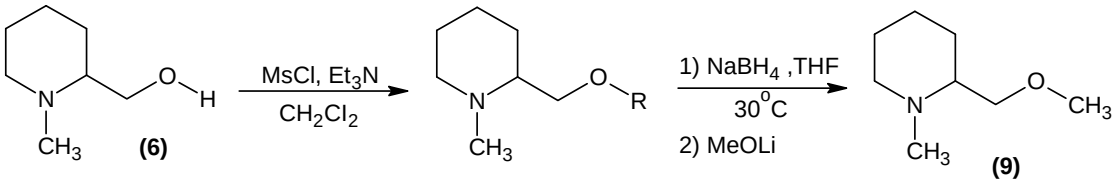
Scheme 4: Methyl Iodide Ether

Another difficulty in isolating any possible product was the excess dimethylformamide (DMF) present after several workups. The use of other possible solvents included tetrahydrofuran (THF) and diethyl ether reported by Bream et al.[16] proposed using THF in Williamson ether synthesis, which would lower the polarity in comparison to the use of DMF as a medium.[16] THF and ether were used in the same reaction using bromoethane in which less polar spots were visualized with TLC. LC/MS and NMR verified the presence of the desired product with the starting material in excess. It was decided to reproduce the results of the reaction using a diethyl ether medium, with a higher equivalency of the alkyl halide.

Crown ether was used by Aspinall et al. to produce a Williamson ether products from hindered alcohols.[17] The bromoethane substrate was used and produced a crude slurry mixture. The use of bromoethane was attempted again using iodomethane and the crude slurry was treated with HCl/ether to induce crystallization by a procedure noted by Dr. Scott Furness.[18] Another attempt using the ether medium and both alkyl halides was used in which the sodium hydride, alcohol, and reagent were each concentrated with ether before addition to the reaction mixture.

With continuous failure of either product formation or isolation of the desired material, it was decided to transform the hydroxyl group into a mesyl group to enhance S_N2 reactivity. Albrecht et al. performed a protection reactions using mesylchloride.[19] In our experiments, the mesyl chloride and triethylamine were used to create the derivative alcohol using dichloromethane as the medium instead of DMF, ether, or THF (Scheme

5). This was also attempted with tosyl chloride and followed by a replacement by a litium methoxide.



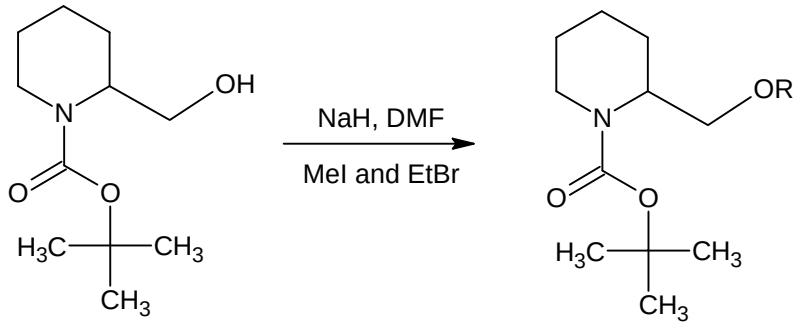
Scheme 5: Tosyl/Mesyl Ethers

After consultation with thesis committee members, it was determined that the reaction should be run again but closely monitored with slight alterations in synthetic techniques, such as making sure the solvents are maintained under anhydrous conditions. The reaction conditions were altered to include addition of the sodium hydride and ethylbromide at 0^{o}C to control the reactivity of the substrates in order to prevent an instantaneous reaction that could possibly lead to unwanted by-products. Additional sodium hydride was added to react with any water that could possibly be present, and still allow enough to react with the alcohol. GC/MS was used to monitor the reaction which yielded the presence of starting material. This reaction was repeated with DMF and analyzed with GC/MS and NMR to yield the same results, without the presence of starting material. This reaction was attempted again with a temperature change in which the mixture was heated to 80^{o}C for 3 hour. An additional equivalency of bromoethane was added and the reaction continued until completion. This was also performed with the iodomethane without the additional methyl iodide. Both reactions did not produce the desired products, which was determined by NMR and GCMS.

The final attempt at producing the ether molecule required a change in the starting material. Perhaps the tertiary nitrogen was undergoing alkylation to give unwanted side products. It was proposed by a colleague to perform the reaction using a protected form of the piperidine moiety. Relying on previous experience with similar molecules, it was concluded that the previous reactions were less likely to form desired material due to possible formation of quarternary ammonium compounds via N-alkylation. The possibility of forming the ether from the previous methodologies is still possible, although purification would be very difficult due to the polarity of the compound. The idea behind using a protected piperidine is to lower the basicity of the nitrogen in the ring. The proposed reaction is a two step reaction where each step can be performed in a one pot synthesis. The first step consists of the formation of the alkoxide using sodium hydride and an aliphatic compound. This material may, or may not, need to be purified. The second step consists of removing the BOC protecting group with either HCl/ether or TFA. Once this has been monitored and verified as deprotected, a methyl group can be added to the nitrogen using various steps. One suggested method is the use of sodium borohydro triacetic acid and formaldehyde in dichloromethane (DCM). If the initial reaction is to be performed successfully, the use of an aromatic instead of aliphatic compound will render the desired products. The aromatic compound will eliminate the possibility of quartenary and intramolecular formation.

The reactions utilizing the Boc-protected piperidine were similar to those performed where the sodium hydride and alkyl halide were separately added at 0^{o}C under argon (Scheme 6). The temperature was increased to 70^{o}C, and the mixture continued to

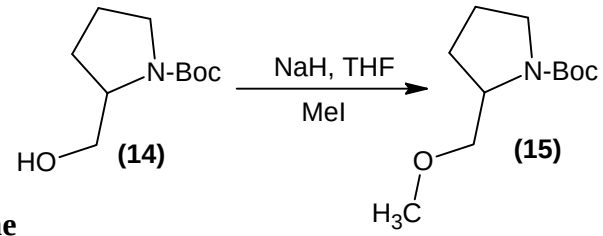
run until completion; however, the desired product was not detected. In a final modification of the reaction, it was repeated with a quick one hour reaction time on a small scale. The alcohol, DMF and sodium hydride were added and allowed to run at 0°C for five minutes before the addition of the ethyl bromide, which only stirred for ten minutes. This still did not yield the desired material which as determined by NMR. LC/MS analysis proved the presence of an excess amount of the starting material and the TLC displayed spots that were more polar, instead of less polar, than that of the starting material.



R=Me **(12)**, Et **(13)**

Scheme 6 N-Boc Ethers

At this time, another procedure was discovered on similar structures but with a pyrolidine instead of a piperidine (Scheme 7).[20] A small scale reaction was set up according to the new procedure, and the reaction was run at room temperature for up to sixteen hours. The TLC of this reaction did not indicate complete transformation of the starting material to the ether, which led to the decision to remove approximately half of the material and allow it to react at 80°C until completion.



Scheme 7 N-Boc pyrollidine

After several attempts using different conditions for various references, it is concluded that possibly the reaction is best performed with the latest procedure[20] containing the Boc protected nitrogen group. The next step will be to perform the same reaction using an aromatic instead of aliphatic group. Once the procedure is successful, it will be further optimized to eliminate steps and improve yields.

Experimental Data

General Procedures. Anhydrous conditions were utilized, and the atmosphere was under Argon. Total consumption of the starting material was monitored by thin layer chromatography (TLC) and the workup is designated under each procedure. The TLCs were developed with the required solvent polarity and visualized with phosphomolybdic acid (PMA), iodine crystals, or UV light. The organics recovered from the work up were dried anhydrous over sodium sulfate (Na_2SO_4) or magnesium sulfate (Mg_2SO_4), and the solvent removed through rotary evaporation. Flash column chromatography on silica gel was performed to purify the crude material. The products were analyzed by proton and carbon NMR with deuterated chloroform as the reference. Certain selected reactions were analyzed using GC/MS and LC/MS.

1-methyl-2-[(1-methylpropoxy)methyl]piperidine (1).

1. Sodium metal in mineral oil (0.48g, 18 mmol) was added to a flask and cooled to 0^oC. 4 mL of anhydrous DMF was added and the mixture stirred at 0^oC for five minutes before addition of n-methylpiperidine methanol (1.94g, 15 mmol) via syringe. The reaction flask was then removed from the ice bath and continued to stir under argon at room temperature for 1 h. sec-Butyl bromide (2.06g, 15 mmol) in DMF was added, and the reaction continued to stir at room temperature for 2.5h at which time ethyl acetate and water were used to quench and workup the crude product.

2. sec-Butyl bromide and sodium hydride (in mineral oil) were added to a solution of n-methylpiperidine-2-methanol and DMF. The mixture was set to reflux overnight under argon. An additional amount of DMF (5 mL) was added to the mixture after 2 hours, and the reaction continued to stir for a total reaction time of 18 h. Ethyl acetate and water were used to quench and workup the reaction. The organics were dried over potassium carbonate (K_2CO_3), and the solvents evaporate to yield a brown oil.

2-(ethoxymethyl)-1-methylpiperidine (2).

1. The alcohol (1.29 g, 10 mmol) and 14 ml of DMF were added to a flask, and sodium metal (0.17g, 7 mmol) was added at 100^{o}C. The temperature of the solution was raised to 140^{o}C, at which time bromoethane (0.98g, 10 mmol) was added. The mixture was allowed to stir overnight under argon at this temperature. The reaction was complete after 24.5 h and was quenched with ethyl acetate and water. The organics were dried over potassium carbonate, and the solvents evaporated to yield a crude brown oil.
2. The reaction was reproduced with a temperature alteration that consisted of a reduction in temperature to RT for 2.5 h before heating to 70^{o}C and allowing to stir overnight.
3. Sodium hydride (0.48, 18 mmol) and 14 mL of DMF were cooled to 0^{o}C to which the piperidine alcohol was added and stirred for 5 min. The mixture was warmed to RT and stirred for 1 h, to which a solution of DMF and ethyl bromide (1.94g,

15 mmol) was added. The mixture was allowed to stir overnight under argon, was quenched with ethyl acetate, and worked up with ethyl acetate and water; then dried over potassium carbonate.

4. The alcohol (1.26g, 10 mmol), ethyl bromide (1.59g, 10 mmol), sodium hydride (0.22g, 7 mmol), and 6 mL of DMF were added to a flask and refluxed under argon overnight. The mixture was quenched with ethyl acetate; the organics extracted with water and then dried over potassium carbonate.
5. The alcohol (0.165g, 1.28 mmol), ethyl bromide (0.064g, 0.64 mmol), and 6 mL of DMF were allowed to stir at 125^{o}C for 40 min, at which time sodium hydride (0.062g, 2.56 mmol) was slowly added. A second portion of sodium hydride (0.068g, 2.56 mmol) was added after 1h and continued to stir at 125^{o}C for 2 h. The heat was reduced, and the mixture stirred for 30 min at RT at which time the reaction was quenched with sodium bicarbonate. The organics were extracted with dichloromethane and washed with saturated sodium chloride. The organics were dried over sodium sulfate, and the solvent evaporated to yield a brown oil.
6. The alcohol (0.168g, 1.30 mmol), 4.8 mL of DMF, and sodium hydride (0.079, 2.56 mmol) stirred for 1h at RT before the addition of the ethyl bromide (0.179g, 1.56 mmol). The reaction continued to stir under argon until completion, at which time saturated sodium bicarbonate was added and stirred for 15 min. The organics were extracted with dichloromethane, washed with brine, and dried over sodium sulfate. The solvents were evaporated to yield a crude reddish/brown oil.

7. The alcohol (0.180g, 1.39 mmol) and 4.8 mL of DMF were refluxed at 120^{o}C before the addition of sodium hydride (0.071g, 2.56 mmol) which stirred for 1 h. The ethyl bromide (0.182g, 1.67 mmol) was added at 110^{o}C and stirred until completion. The cooled reaction was quenched with sodium bicarbonate and stirred for 15 min before being extracted with dichloromethane, washed with brie, and dried over sodium sulfate. The solvents were evaporated to yield a crude reddish/brown oil.
8. Sodium hydride (0.36g, 15 mmol) and 9.4 mL of THF stirred for 5 min before a mixture of the alcohol (0.94g, 7.32 mmol) and 4.7 mL of THF was added dropwise. This mixture stirred at RT for 2 h. At this time, ethyl bromide was added dropwise, and the mixture continue to stir at RT for 1h. The reaction was set to reflux and stirred for an additional 2 h. The organics were extracted with ether and dried over sodium sulfate and concentrated to yield a crude yellow oil.
9. This reaction was run a second time with ether as the solvent instead of THF.
10. Sodium (0.35g, 15 mmol) in 4.8 mL of ether stirred for 5 min, at which time the alcohol (0.96g, 7.30 mmol) in 9.7 mL of ether was added, followed by crown ether (1.83 mL, 8.32 mmol). The mixture stirred for 2 h, then ethyl bromide (1.9g, 10.95 mmol) was added dropwise. The mixture continued to stir at RT until completion. Brine was added and the organics were extracted with ether, then dried over sodium sulfate. The concentrated crude oil was dissolved in a small amount of ether, and HCl in ether was added via pipette. The solvent was evaporated and additional ether was added to generate crystals by swirling flask.

11. Sodium hydride (0.36g, 15 mmol) and 4.83 mL of ether stirred before the addition of 9.7 mL of ether and alcohol (0.95g, 7.3 mmol). This mixture stirred for 2 h at RT before the addition of bromoethane (0.96g, 8.8 mmol). An additional amount of 4 mL of ether was added after 3 h, and the mixture was allowed to stir for the remainder of the 2 h period. The mixture continued to stir for 2 h after addition of bromoethane and was quenched with brine. The organics were extracted with ether and dried over sodium sulfate. They were concentrated to yield a yellow oil. Ether was added, followed by hydrogen chloride saturated ether to induce crystallization. This solution sat for 15 min, then was evaporated to yield a yellow solid. Ether was added and the solution swirled for 15 min, then was allowed to sit open to atmosphere overnight. This process was done twice to induce crystallization of the material.
12. The alcohol (0.394g, 3.05 mmol) and 4 mL of THF were cooled to 0^{o}C under argon for 5 min. Sodium hydride (0.152g, 6.1 mmol) was then added, and the mixture was warmed to RT and stirred for 15 min. The mixture was cooled 0^{o}C and ethylbromide (0.665g, 6.1 mmol) was added dropwise. The reaction was warmed to RT and continued to stir for 4.5 h. Ethyl acetate was added, followed by the slow addition of water. The organics were extracted with ethyl acetate and dried over magnesium sulfate. The solvent was evaporated to yield a crude yellow oil.
13. This reaction was reproduced with the use DMF as a solvent.

14. The reaction was again run using DMF, with a change in temperature settings. The alcohol (0.300g, 2.32 mmol) and 4 mL of DMF were added and stirred for 5 min under argon at 0^{o}C. The sodium hydride (0.111g, 4.64 mmol) was added; the mixture was warmed to RT and stirred for 1 h under argon. Bromoethane (0.506g, 4.64 mmol) was added dropwise at 0^{o}C, and the mixture was warmed to RT and stirred for 1h. The mixture was then heated to 80^{o}C for 3h, at which time an additional 2 equivalents of bromoethane was added dropwise. The mixture continued to stir at 80^{o}C for another 3h and 15 min. Dichloromethane and water were used to quench the reaction. The organics were extracted with dichloromethane and dried over magnesium sulfate. The solvent was evaporated to yield a crude yellow oil.
15. This reaction was reproduced with the same solvent and temperature settings and methyl iodide (0.659g, 4.64 mmol) as the substrate.

2-(methoxymethyl)-1-methylpiperidine (3).

1. The alcohol (0.176g, 1.28 mmol) and 4.8 mL of DMF stirred at RT for 10 min before the addition of sodium hydride (0.068g, 2.56 mmol), and the mixture was allowed to stir for 1 h. Methyl iodide (0.224g, 1.54 mmol) was added and stirred for 2 h at RT, then the reaction mixture was quenched with sodium bicarbonate which stirred for 15 min. The organics were extracted with dichloromethane, washed with brine, and dried over sodium sulfate. The organics were

concentrated to yield a light yellow oil. The reaction was repeated with sodium hydride being added at 120^{o}C and the methyl iodide stirred at 110^{o}C.

2. The sodium hydride (0.41g, 15 mmol) and 5 mL of ether stirred for 5 min, at which time the alcohol (0.94, 7.3 mmol) dissolved in 9.7 mL of ether was added dropwise. This mixture stirred for 2 h at RT. The methyl iodide (1.25g, 8.8 mmol) was added, and the mixture continued to stir until completion of reaction. Brine was added, and the organics were extracted with ether. The organics were dried over potassium and concentrated to yield a crude yellow oil.

(1-methylpiperidin-2-yl)methyl methanesulfonate (4). The alcohol (0.78g, 6.0 mmol), 10 mL of dichloromethane, and triethylamine (1.9 mL, 13.8 mmol) were stirred under argon at 0^{o}C for 5 min, at which time the mesylchloride (0.57 mL, 7.2 mmol) was added dropwise. This mixture continued to stir for 1 hr before being quenched with ammounium chloride, extracted with dichloromethane, and dried over magnesium sulfate. The solvents were then evaporated to yield a crude oil.

(1-methylpiperidin-2-yl)methyl 4-methylbenzenesulfonate (5). The alcohol (0.78g, 6.0 mmol), triethylamine (1.9g, 13.8 mmol), and 10 mL of dichloromethane were added and placed under argon at 0^{o}C, at which time tosyl chloride (0.88g, 7.2 mmol) was added. The mixture continued to stir under argon for 1.5 h before ammonium chloride was used to quench the reaction. The organics were extracted with dichloromethane and washed

with sodium chloride. The organics were dried over magnesium sulfate, and the solvents evaporated to yield a crude yellow oil and some white crystals.

2-(methoxymethyl)-1-methylpiperidine (3). The tosylate (0.31g, 1.09 mmol), sodium borohydride (0.102g, 2.19 mmol), and 8 mL of THF were added to a flask and allowed to stir at RT for 2 h. Lithium methoxide (0.113g, 2.19 mmol) was added after the reaction stirred for 2 h, and the mixture was allowed to stir for an additional 2 h. Water was used to quench the reaction, ether was used for the extraction, and the organics were dried over sodium sulfate and evaporated to yield light a yellow oil.

***tert*-butyl 2-(methoxymethyl)piperidine-1-carboxylate (6).** The alcohol (0.500g, 2.32 mmol) and 4.2 mL of DMF were stirred at 0^{o}C prior to the addition of sodium hydride (0.120g, 4.64 mmol). The mixture continued to stir at RT under argon for 1 h. Methyl iodide (0.659g, 4.64 mmol) was added at 0^{o}C, and the mixture was warmed to RT and stirred for 1 hr. The temperature was raised to 70^{o}C and continued to stir until an additional equivalent of methyl iodide was added and the reaction continued to stir at 60^{o}C until completion. Water and dichloromethane were added to quench the reaction. Dichloromethane was used to extract the organics which were dried over magnesium sulfate. The solvent was evaporate to yield a reddish brown oil.

***tert*-butyl 2-(ethoxymethyl)piperidine-1-carboxylate (7).** The alcohol (0.100g, 2.32 mmol), 2 mL of DMF, and sodium hydride (0.50g, 11.6 mmol) stirred for 5 min at 0^{o}C, at

which time the ethyl bromide (0.659g, 4.64 mmol) was added and stirred for 10 min before being worked up with methanol. The organics were extracted with water and ether and dried over magnesium sulfate. The solvent was evaporated to yield a crude yellow oil.

CHAPTER II

COMPUTATIONAL STUDIES OF SOLENOPSIN A ANALOGS

Introduction

Computational chemistry has developed over an extended period of time, and it may now be considered one of the main branches of chemistry. The origins may be traced in part to molecular modeling in the form of handheld mechanical models. The importance of visualizing molecular structures extends beyond simply understanding the atomic connectivity to include energy, physical properties, and possible interactions with other molecular systems. Investigating these properties may lead to a better understanding of a molecule's potential as a possible drug lead, as well as synthetic feasibility. Structure activity relationships (SARs) can be predicted and used in drug design. One example of a beneficial development in computational chemistry methodology has been the calculation of relative free energies of inhibitors binding to HIV-1 protease.[21] The interactions were estimated through use of hydrophobic surface property maps between the inhibitors and binding sites of the protease.[21]

Molecular visualization finds a natural and central place in medicinal chemistry research. Implementing calculations for specific products or transition state molecules have assisted medicinal chemists to design potential therapeutic agents. Computational chemistry predictions may be derived from structural-based determination of ideal

molecules in which the lowest energy is calculated along with chemical properties (e.g. NMR chemical shifts, ionization potentials, and electronic spectra).[22]

The use of structure based drug design, where appropriate, is also an important goal for medicinal chemists to develop potential drug candidates. The ability to visualize properties aids in the molecular design process.[21] Utilizing molecular modeling can assist in the avoidance of wasted efforts in time and money preparing unrealistic synthetic targets. The concept of molecular modeling involves the use of molecular design and computational studies to predict properties essential for drug receptor interactions, such as molecular geometries, energetic, chemical reaction pathways, ADME (absorption, distribution, metabolism, elimination), and biological responses (CADD) and usually involves simplifying approximations of a more general theory to extend its practical utility.[22] Computational chemistry developments allow for more accurate calculations due to the increase of computer speeds and more reliable potential energy functions.[21]

Quantum and molecular mechanics are the foundations of computational chemistry. These calculations are used to study potential drug candidates *in silico*. Both computational methods are based originally on gas phase equations, where each Individual approach is separately applied according to the specific calculation requirements, which can include the geometry, energy, surface area, dipole moments, etc. The selection of an appropriate method is determined by the size of a particular molecular system and the research goals. Larger molecules are best investigated with molecular

mechanics, while a smaller system uses quantum mechanical calculations.[22] Quantum mechanics consists of three different methods, *ab initio*, density functional theory (DFT), and semi-empirical methods. *Ab initio* which is Latin for "from the beginning" involves calculations that are solely based on theory and not experimental application, although there are some simplifying approximations. Density functional theory investigates electronic structures through properties that are derived from the use of electronic density function. Semi-empirical methods consist of brutal approximations, which omit key integrals that leads to calculations which are faster than *ab initio*, but the answers are crude and only qualitative at best. Overall, applications are used for a particular calculated problem.

Alternatively, molecular mechanics is particularly suited for drug design investigations, and it is the basis for many CADD methods. It may be defined as a mathematic approach used to calculate the structures and associated energies of molecular systems.[23] The force field, which is a set of parameters and equations used to determine the potential energy of a molecule, yields desired information about physical properties that may lead to insight into the bioactive conformations. A fundamental concept in molecular mechanics is the distribution of the total energy of a molecular system into potential functions associated with bending, stretching, and nonbonded energies.

Medicinal chemists use computational chemistry to better understand lead-target interactions. Understanding bioactive conformations involves gathering information

from different aspects, such as structure-function relationships.[24] An economic motivation for using computational methods is to explore molecular properties prior to experimental work. The goal is to minimize the time and expense of laboratory preparations and evaluations. The uses of computational chemistry extend beyond the calculation of gas phase molecular structures to include energetically favorable conformations and ADME/Tox properties.

The piperidine moiety has proven important throughout chemical history as a biologically active unit. Further exploration can only continue to prove itself more useful. This valuable heterocycle has been studied and decided through experimental investigation to be clinically useful in treating infections, schizophrenia, and Parkinson's disease; as well as a more recent discovery of its functions with cocaine abuse medications.[25] Due to the various applications of the synthetic compounds that consist of the piperidine component, necessary molecular modeling calculations have been carried out to further investigate the properties of piperidines and its derivatives.

Important studies were undertaken that focused on the nitrogen and the placement of methyl substituents on different ring positions. These are important to the investigation of solenopsin A analogs which contain some form of the previously investigated compounds. The piperidine ring was studied with emphasis placed on the nitrogen moiety by Lobato-Garcia, et al. who focused on the conformational energies.[26] The importance of focusing on a molecule's ability to alter its conformational states provides insight into its binding affinity and affords the lowest possible energy of the

molecule.[21] Three noteworthy items were observed in this study: quantum chemical *ab inito* calculations have afforded relation between nitrogen inclusion and biological effects; "polarized basis sets" are also useful for the conformational studies; *ab initio* and density functional theory (DFT) were used to calculate minimum energies and thermodynamic properties. The conformational distributions energies were calculated using the Monte Carlo method, of which further minimization was completed using the B32YP method and 6-311G basis set. These conformers were selected for each compound in question to yield a conclusive presentation of a chain conformation of the 6-membered piperidine ring. There are some important observations from the data, such as the equatorial position of the substituents on nitrogen in the piperidine is referenced as being "generally accepted by 6-membered saturated cycles".[26] An important observation is the interaction of the oxygen within the "spatial proximity" of the hydrogen, which is indicative of weak intramolecular hydrogen bonding. The interaction between the nitrogen and hydrogen is also significant in the illustration of conformational energy stability. The dihedral angles were also investigated to further support the conclusion concerning the stabilities of the conformers. The conclusion from the Lobato-Garcia study attributes the conformational differences to the "spatial disposition of substituents", with noted interest on the "diasterotopic hydrogen" of these conformers.[26]

Another important study concerning the piperidine moiety was done by Ribiero de Silva et al., who focused on the thermochemistry and conformational stability of methylpiperidines.[25] The energy of combustion investigation of these derivatives

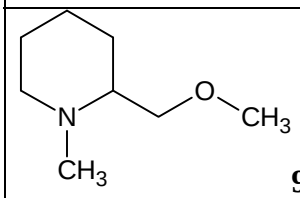
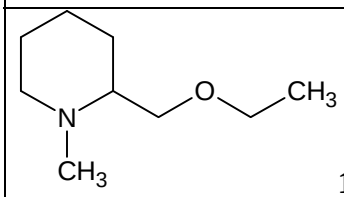
consisted of obtaining commercially available samples of the methyl piperidines which were measured by combustion calorimetry: 1-methylpiperidine, 3-methylpiperidine, 4-methylpiperidine, 2,6-dimethylpiperinde, and 3,5-dimethylpiperidine. The relevance of this study is fueled by the published work that analyzes the conformational stability of piperidine derivatives. The thermochemistry work has also been investigated for this motif by utilizing computational theories, such as *ab initio* and DFT. In de Silva's particular study, only the axial conformers were considered; they were found to be less stable than equatorial, which was also shown in the results of Lobato-Garcia et al.[26] De Silva's work also proved that the MP2/6-31G* method is a more accurate approach to investigate piperidine conformers. With this additional motivation for the study, the methyl piperidine derivatives were investigated using MP2, BP86, and B3LYP methods with the 6-31G(d) basis set. The study illustrated the stabilities of the derivatives in comparison with the axial and equatorial conformations. It was concluded that "all compounds are more stable when in the equatorial and chair conformations".[25] The geometrical calculations also afforded results "suggesting the space occupied by [the] methyl group is smaller than an unsubstituted nitrogen in the piperidine ring".[25] The calculation of the enthalpy of formation is in agreement with the results of the conformational studies. The results from this study lead to a conclusive determination that the ring is more stable with nitrogen unsubstituted and the varying placements of methyl groups around the ring.

Results and Discussion

Computational chemistry techniques were employed to gain insight into conformational preferences for the piperidine ether analogs. Each structure was calculated using quantum and molecular mechanics in Spartan. The calculations were carried out using the equilibrium geometry options and the Hartree-Fock model with the 6-31G* basis set. Each structure was subjected intially to a molecular mechanics conformer search, followed by quantum mechanical calculations of the lowest energy conformers (Table 2). The dihedral angles were recorded for each conformer, and again for the minimized conformers. These molecules have been compared to solenopsin A to establish some understanding of the role the oxygen plays in conformational stability and the interconversion of one conformer into another. The molecules submitted for energy calculations include N-substituted and non-substituted piperidines. The substituents on the oxygen and nitrogen moieties vary from simple ethyl chains to aromatic groups (Table 1). The molecules in the first set of calculated energies include substituted and non-substituted piperidines with the methyl oxygen ethers: **9,** 2-(methoxymethyl)-1-methylpiperidine; **16**, 2-(ethoxymethyl)-1-methylpiperidine;**17**, 2-(methoxyundecyl)-1-methylpiperidine; **18**, (1-methylpiperidin-2-yl)methyl methanesulfonate; **19**, (1-methylpiperidin-2-yl)methyl 4-methylbenzenesulfonate; **20**, 2-(methoxymethyl)piperidine; **21**, 2-(ethoxyethyl)piperidine; **22**, 2-(methoxyundecyl)piperidine;**23**, 2-(piperidin-2-yl)methyl methanesulfonate; **24**, piperidin-2-ylmethyl 4-methylbenzenesulfonate.

The second data set includes commercially available compounds and their desired synthetic products: **25**, N-boc-piperidine-2-methanol; **26**, N-boc-piperidine-2-ethanol; **27**, N-boc-piperidine-2-ethoxymethyl; **28**, N-boc-piperidine-2-ethoxymethyl. Commercially available derivatives were purchased for biological testing: **29**, 2-(2-methoxyethyl)piperidine; **30**, 2-(2-ethoxyethyl)piperidine; **31**, 2-[2-(benzyloxy)ethyl]piperidine; **32**, 2-(2-propoxyethyl)piperidine; **33**, 2-[2-(3-phenylpropoxy)ethyl]piperidine. The fourth set consisted of a nitrogen instead of oxygen moiety: **34**, *N*,*N*-diethyl-2-piperidin-2-ylethanamine; **35**, *N*,*N*-dimethyl-2-piperidin-2-ylethanamine; **36**, 4-methyl-1-(2-piperidin-2-ylethyl)piperidine; **37**, 1-(2-piperidin-2-ylethyl)piperidine; **38**, 1-(2-piperidin-2-ylethyl)azepane; **39**, 2-(2-pyrrolidin-1-ylethyl)piperidine. All of the analogs are derived from the solenopsin A lead structure: **40,** *trans*-2-methyl-6-*n*-undecylpiperidine.

Table 1: Molecular Modeling Structures

Structure
 **9**
 **16**

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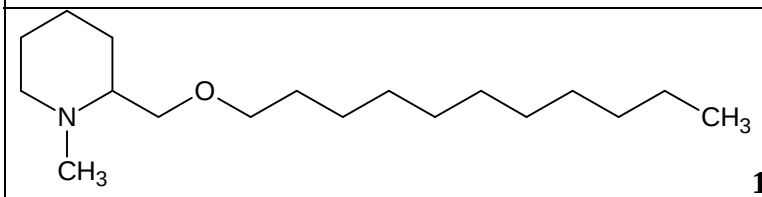

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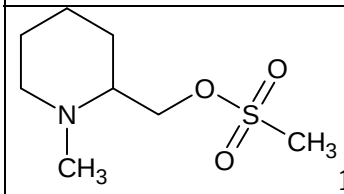

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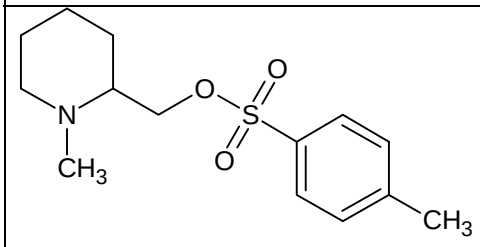

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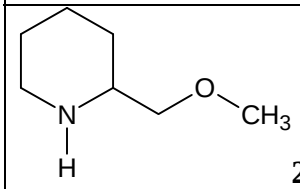

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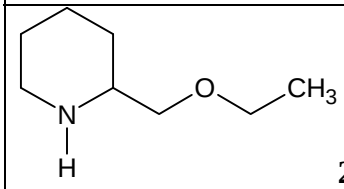

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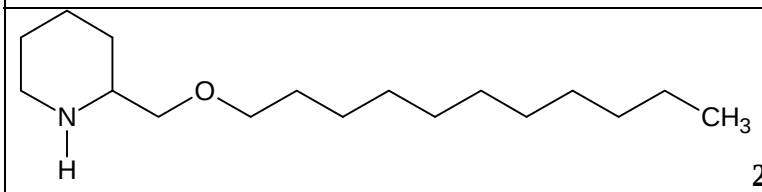

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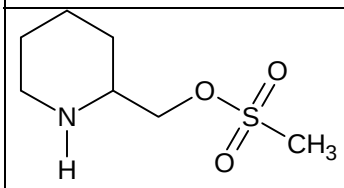

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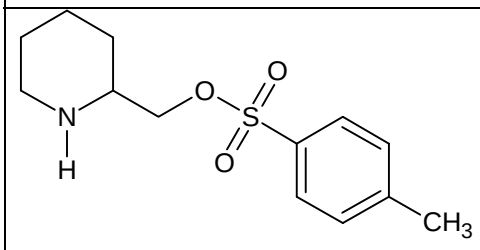

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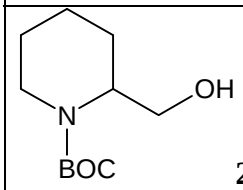

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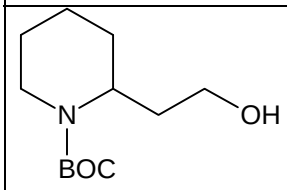

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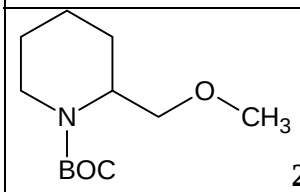

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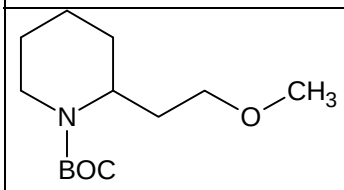

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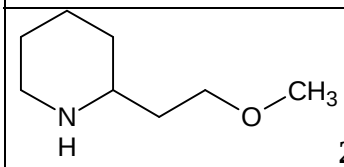

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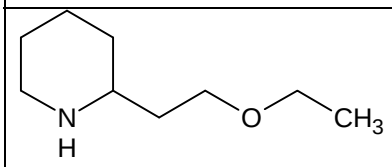

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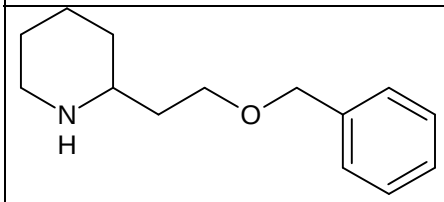

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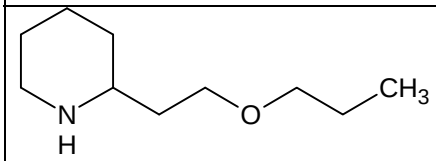

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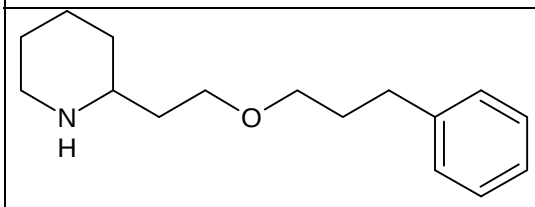

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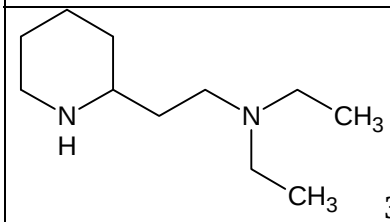

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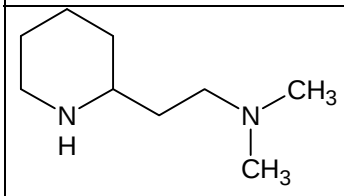

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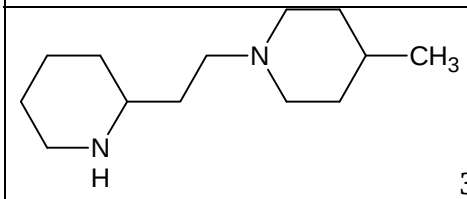

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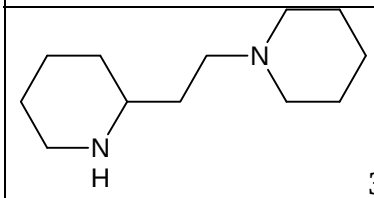

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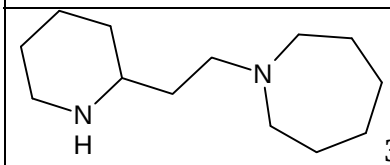

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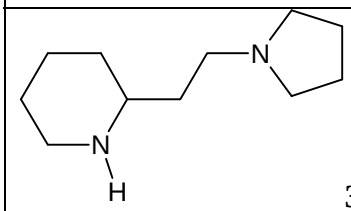
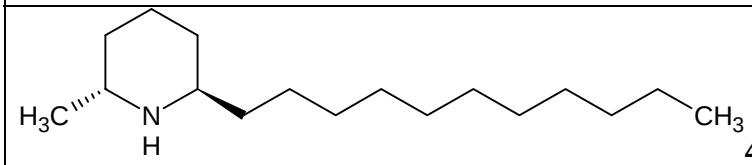


39



40

The first set of molecules, **1** through **10,** to undergo energy calculations consisted of substituted and un-substituted piperidine molecules where the side chain contains an oxygen with various alkyl groups. The lowest energy molecule in the set of un-substituted and methylated piperidines is the tosylate protected oxygen, with quantum energies of -1179.82 au and -1218.85 au, respectively. As expected, the lowest energy conformer of each molecule in the first data set for both piperidine groups illustrate that the methyl-substituted nitrogen of the piperidine moiety produces a lower quantum energy value. Solenopsin A has a HF energy of -718.61 au for its lowest energy

conformer. The lowest conformer energies are shown in relation to the lowest relative energies (Table 2).

Failure to produce results from the initial synthesis of the Williamson ether compound from 2-piperidine methanol led to the investigation of another substrate, N-boc-piperidine-2-methanol. **11** was utilized in the lab and also submitted for energy calculations through molecular modeling. The second data set consists of the two commercially available Boc-protected piperidines (**11**,**12**) and the desired alkylated ether products (**13**,**14**) (Table 1). The methyl component of the starting material and product yielded HF energies of -707.84 au and -746.86 au, respectively. The ethyl component afforded -746.87 au and -785.89 au for the starting material and product. The lowest energy conformers of each molecule were calculated using the Hartree-Fock method (Table 2).

The third and fourth data sets are a combination of commercially available derivatives, some of which have been purchased and submitted for biological testing against the Akt enzyme for anti-angiogenic activity using the SVR assay. The molecules in the third data set still contain the oxygen functionality and a non-substituted nitrogen, with variations in the chain which include aliphatic and aromatic groups (**15-19**). The lowest energy molecule calculated is the 2-(3-phenylpropoxy)ethyl piperidine of -749.75 au (Table 2). All of these molecules, with the exception of 2-benzyloxyethylpiperidine (**17**), have been submitted for biological testing with pending results.

The fourth, and final, data set consists of a nitrogen in place of an oxygen moiety (**20**-**24**). Only two items from this set were purchased and submitted for testing with pending biological results: diethyl-2-piperidine ethyl amine, **20**, and dimethyl-2-piperidine methyl amine, **21** (Table 1). The minimized conformers have been listed with their relative energies. No comparison has been made, but the data has been collected for possible use in further investigations (Table 2).

Table 2: Conformer Relative Energies

Structure Number	**Conformer 1**	**Conformer 2**	**Conformer 3**	**Conformer 4**	**Conformer 5**
9[a]	0.0030	0.0000*	0.0046	0.0052	N/A
16[b]	0.0000*	0.0019	0.0030	0.0026	0.0026
17[c]	0.0000*	0.0001	0.00197	0.0040	0.00207
18[d]	0.0006	0.0009	0.000*	0.0010	0.0029
19[e]	0.0012	0.000*	0.0010	0.0007	0.0012
20[f]	0.000*	0.0030	0.0040	0.0070	0.0010
21[g]	0.000*	0.0024	0.00257	0.002581	0.000*
22[h]	0.0002	0.000*	0.0015	0.0019	0.0017
23[i]	0.000*	0.0030	0.0020	0.0060	0.0060

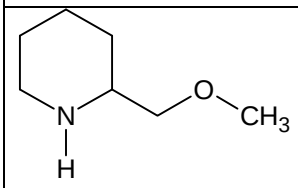
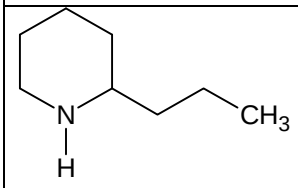
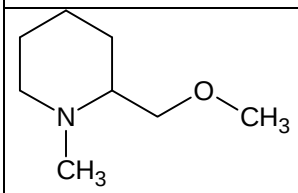
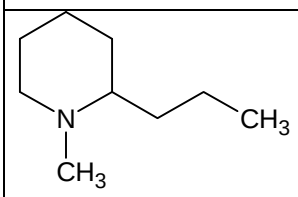
24[j]	0.000*	0.00170	0.00160	0.0050	0.0032
25[k]	0.000*	0.002943	0.002942	0.00689	N/A
26[l]	0.00149	0.000*	0.00170	0.000798	0.00192
27[m]	0.000*	0.002446	0.005050	0.007948	0.00804
28[n]	0.000155	0.0011	0.000*	0.002729	0.003728
29[o]	0.000*	0.000868	0.002737	0.003342	0.001681
30[p]	0.000*	0.000871	0.002603	0.002715	0.002635
31[q]	0.000*	0.000214	0.000388	0.003466	0.001105
32[r]	0.000285	0.000149	0.000082	0.000236	0.000*
33[s]	0.000106	0.0001	0.001489	0.001508	0.000*
34[t]	0.003011	0.003679	0.004057	0.000*	0.001952
35[u]	0.000*	0.00027	0.001049	0.002008	0.001965
36[v]	0.001971	0.000*	0.001971	0.004087	0.005715
37[w]	0.000*	0.000931	0.00200	0.005372	0.006304
38[x]	0.001925	0.003584	0.002154	0.000*	0.001018

39[y]	0.000*	0.000249	0.001914	0.005209	0.006531
40[z]	0.000*	0.00020	0.0017	0.0016	0.0021

*a: 2, -442.1250 au; b: 1, -481.1648 au; c: 1, -832.479 au; d: 3, -989.3086 au; e: 2, -1218.8538 au; f: 1, -403.101 au; g: 1,5, -442.1409 au; h: 2, -793.4569 au; i: 1, -950.286; j: 1, -1179.8173 au; k: 1, -707.84729 au; l: 2, -746.87119 au; m: 1, -746.86715 au; n: 3, -785.8997 au; o: 1, -442.13576 au; p: 1, -481.17579 au; q: 1, -671.684248 au; r: 5, -520.21078 au; s: 5, -749.75684 au; t: 4, -539.403226 au; u: 1, -461.33439 au; v: 2, -616.31814 au; w: 1, -577.2840 au; x: 4, -616.307361; y: 1, -538.24355; z: 1, -718.6100 au

The dihedral angles were recorded for each molecule and the individual energy conformers were submitted for quantum calculations. The torsion angles relate to the chemical bonds that intersect the plane, while the bond angles relate to the electronic pairs in the valence shell. The independent parameters that are visualized correlate to conformations such as chair, which is almost free of strain and boat, which is free of angle strain. There are some noticeable differences in the dihedral angles of the minimized conformers, although a direct comparison or conclusion has not been determine. The dihedral angles of methylated and non-substituted piperidines with the oxygen and carbon moieties were investigated and the initial angles were documented, followed by the parameters of the minimized conformers, which are in parentheses preceding the original conformer values. These values were calculated at the set dihedral angles of 30^{o}, 60^{o}, 90^{o}, 120^{o}, and 180^{o} (Table 3).

Table 3: Dihedral Angle Data

Structure	Energy (au) 30°	Energy (au) 60 °	Energy (au) 90 °	Energy (au)120 °	Energy (au)180 °
	-403.0993	-403.0993	-403.0993	-403.0993	-403.1021
	-367.2925	-367.2849	-367.2925	-367.2942	-367.2942
	-442.1236	-442.1236	-442.1248	-442.1263	-442.1263
	-406.3162	-406.3129	-406.3162	-406.3178	-406.3179

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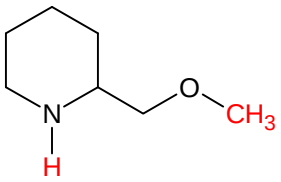
APPENDIX

COMPUTATIONAL DATA

Compound 20



Molecule (-403.10 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	22.79356	0
Conformer.2	23.89023	1.09667
Conformer.3	24.53839	1.74483
Conformer.4	25.81579	3.02223
Conformer.5	28.34086	5.5473
Conformer.6	28.47425	5.68069

minimized conformers	mepconf#	Relative Energy (kcal/mol)
Conformer.1	-403.101	0
Conformer.2	-403.098	0.003
Conformer.3	-403.097	0.004
Conformer.4	-403.094	0.007
Conformer.5	-403.100	0.001
Conformer.6	-403.090	0.011

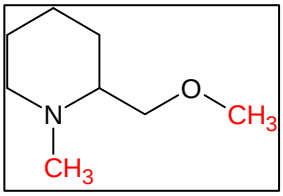
	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
Conformer 1	(52.81) 51.9263	(-52.06) -51.745	(53.05) 55.8437
Conformer 2	(52.89) 52.0037	(-52.24) -52.015	(52.99) 55.8381
Conformer 3	(-52.35) -52.113	(53.76) 52.1869	(-55.66) -54.743
Conformer 4	(-52.37) -52.509	(54.10) 52.5137	(-55.81) -54.625

Conformer 5	(52.76) 53.0312	(-52.65) -51.398	(53.71) 55.1405
Conformer 6	(-52.51) -51.469	(52.97) 51.6152	(-56.08) -55.462

	Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,O1)
Conformer 1	(-54.70) -59.531	(-178.83) -177.7	(175.74) 176.704
Conformer 2	(-54.29) -59.054	(-179.94) -178.51	(179.12) -179.28
Conformer 3	(58.98) 56.9949	(70.89) 71.8734	(171.07) 171.353
Conformer 4	(58.70) 56.3561	(70.96) 72.644	(175.40) 177.864
Conformer 5	(-54.68) -60.292	(179.75) -177.17	(171.66) 142.878
Conformer 6	(61.73) 59.159	(38.91) 69.7338	(135.38) 134.198

*(xxx) relates to the dihedral angles of the minimized conformers

Compound 9



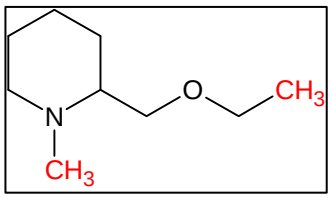
Molecule (-442.13aul)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	32.105773	-0.642508999
Conformer.2	32.748282	0
Conformer.3	34.831071	2.082789
Conformer.4	35.696259	2.947977

minimized conformers (au)		relative energy (kcal/mol)	
Conformer.1	-442.1220	0.0030	
Conformer.2	-442.1250	0.0000	
Conformer.3	-442.1204	0.0046	
Conformer.4	-442.1198	0.0052	
Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
(-179.67) -177.340	(-53.76) -53.934	(54.29) 54.227	(-57.42) -56.972
(-178.09) -176.933	(-53.12) -53.762	(52.35) 52.868	(-56.35) -56.035
(82.84) 80.852	(49.57) 47.478	(-52.93) -49.642	(56.00) 54.220
(-177.71) -176.204	(-54.00) -53.385	(53.87) 53.922	(-56.61) -56.697

Dih(C2,C1,N1,C8)	Dih(C1,N1,C8,C5)	Dih(C8,N1,C5,C6)	Dih(N1,C5,C6,O1)
(-175.77) -178.079	(-125.77) -123.673	(57.89) 58.013	(72.22) 77.307
(-170.34) -175.195	(-127.81) -124.839	(49.04) 54.423	(57.41) 61.390
(77.81) 72.655	(-131.77) -126.826	(145.28) 154.127	(73.44) 78.252
(-174.55) -177.504	(-126.51) -124.343	(51.16) 54.512	(36.31) 34.198

Dih(C7,O1,C6,C5)	Dih(O1,C6,C5,C4)
(-85.84) -85.838	(-52.27) -52.262
(176.90) 176.903	(-66.20) -66.202
(-178.64) -178.636	(-57.00) -57.005
(68.69) 68.694	(-89.66) -89.663

Compound 16



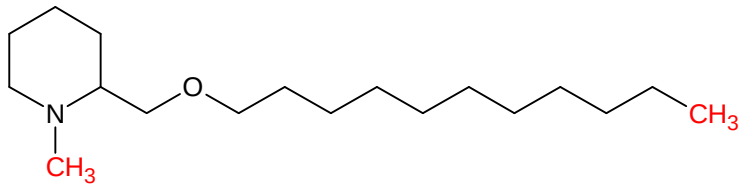
Molecule (-481.165 au)	Egas(kcal/mol)	Rel. Egas (kcal/mol)
Conformer 1	28.94606	0
Conformer 2	29.842155	0.896094999
Conformer 3	30.078489	1.132429
Conformer 4	30.357828	1.411768
5	30.503007	1.556947
6	30.686032	1.739972
7	31.04085	2.09479
8	31.336442	2.390382
9	31.415937	2.469877
10	31.682369	2.736309
11	32.265824	3.319764
12	32.533464	3.587404
13	32.570324	3.624264
14	33.185804	4.23974399
15	35.497538	6.55147799
16	37.397392	8.45133199

minimized conformers nmpe#		relative energies (kcal/mol)
Conformer 1	-481.1648	0
Conformer 2	-481.1629	0.0019
Conformer 3	-481.1618	0.003
Conformer 4	-481.1622	0.0026
Conformer 5	-481.1622	0.0026

Dih(C8,C7,O1,C6)	Dih(C7,O1,C6,C5)	Dih(O1,C6,C5,C54)	Dih(C6,C5,C4,C3)
(179.91) -179.984	(-179.05) 179.323	(-62.82) -57.720	(-75.21) -73.521
(179.70) -179.713	(179.28) -178.526	(-66.32) -62.732	(176.72) 177.363
(178.77) -176.473	(-90.24) -76.717	(-61.14) -51.395	(-75.26) -73.615
(-79.76) -82.833	(-175.64) 178.137	(-63.07) -57.911	(-75.15) -73.406
(78.61) 78.9211	(175.85) 176.111	(-63.11) -57.812	(-75.25) -73.519

Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C9)
(-53.06) -53.041	(52.79) 51.436	(-54.24) -54.003	(-166.55) -173.057
(52.04) 51.402	(-51.25) -51.182	(54.39) 54.262	(75.72) 72.857
(-52.91) -53.385	(52.89) 51.774	(-54.95) -53.972	(-166.61) -173.788
(-53.12) -53.110	(52.79) 51.440	(-54.16) -53.941	(-166.69) -173.159
(-53.02) -53.036	(52.75) 51.414	(-54.25) -53.997	(-166.41) -173.011

Dih(C1,N1,C9,C5)	Dih(C9,N1,C5,C6)	Dih(N1,C5,C6,O1)
(-136.10) -128.559	(-63.99) -59.194	(171.61) 176.857
(-129.54) -126.459	(54.51) 55.439	(165.09) 168.967
(-136.01) -128.383	(-64.17) -58.146	(173.52) -177.120
(-136.13) -128.548	(-64.02) -59.255	(171.40) 176.732
(-136.15) -128.569	(-64.07) -59.238	(171.29) 176.778



Compound 17

Molecule (-832.47 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	25.467395	0
Conformer.2	25.573465	0.10607
Conformer.3	26.242585	0.77519
Conformer.4	26.586159	1.11876
Conformer.5	26.664844	1.19745
Conformer.6	26.753604	1.28621
Conformer.7	26.883468	1.41607
Conformer.8	26.941514	1.47412
Conformer.9	27.128355	1.66096
Conformer.10	27.188595	1.7212
Conformer.11	27.25029	1.7829
Conformer.12	27.335113	1.86772
Conformer.13	27.364056	1.89666

Conformer.14	27.387829	1.92043
Conformer.15	27.419696	1.9523
Conformer.16	27.425772	1.95838
Conformer.17	27.432298	1.9649
Conformer.18	27.487249	2.01985
Conformer.19	27.490835	2.02344
Conformer.20	27.378633	1.91124
Conformer.21	27.681796	2.2144
Conformer.22	27.69354	2.22615
Conformer.23	27.716514	2.24912
Conformer.24	27.788052	2.32066
Conformer.25	27.809584	2.34219
Conformer.26	27.877863	2.41047
Conformer.27	27.759932	2.29254
Conformer.28	27.960189	2.49279
Conformer.29	28.209207	2.74181
Conformer.30	28.247731	2.78034
Conformer.31	28.266604	2.79921
Conformer.32	28.439723	2.97233
Conformer.33	28.41407	2.94668
Conformer.34	28.525284	3.05789
Conformer.35	28.538964	3.07157
Conformer.36	28.563312	3.09592
Conformer.37	28.64869	3.1813
Conformer.38	28.801955	3.33456
Conformer.39	28.968545	3.50115
Conformer.40	29.015213	3.54782
Conformer.41	29.061018	3.59362
Conformer.42	29.377953	3.91056
Conformer.43	29.413483	3.94609
Conformer.44	29.546582	4.07919
Conformer.45	29.673079	4.20568
Conformer.46	29.792069	4.32467
Conformer.47	29.994905	4.52751
Conformer.48	30.018223	4.55083
Conformer.49	30.044266	4.57687
Conformer.50	30.144381	4.67699

Conformer.51	30.196134	4.72874
Conformer.52	30.284006	4.81661
Conformer.53	30.175609	4.70821
Conformer.54	30.372511	4.90512
Conformer.55	30.640503	5.17311
Conformer.56	30.682964	5.21557
Conformer.57	30.812927	5.34553
Conformer.58	30.822241	5.35485
Conformer.59	30.856155	5.38876
Conformer.60	30.955668	5.48827
Conformer.61	31.087691	5.6203
Conformer.62	31.182519	5.71512
Conformer.63	31.385519	5.91812
Conformer.64	31.593603	6.12621
Conformer.65	31.70339	6.23599
Conformer.66	31.894705	6.42731
Conformer.67	3123.4643	3098
Conformer.68	32.184789	6.71739
Conformer.69	32.192694	6.7253
Conformer.70	32.246917	6.77952
Conformer.71	32.25027	6.78287
Conformer.72	32.469786	7.00239
Conformer.73	32.585495	7.1181
Conformer.74	32.620119	7.15272
Conformer.75	32.601492	7.1341
Conformer.76	32.648794	7.1814
Conformer.77	32.734337	7.26694
Conformer.78	32.739353	7.27196
Conformer.79	32.992146	7.52475
Conformer.80	33.084295	7.6169
Conformer.81	33.112302	7.64491
Conformer.82	33.259114	7.79172
Conformer.83	33.362725	7.89533
Conformer.84	33.399948	7.93255
Conformer.85	33.416667	7.94927
Conformer.86	33.642445	8.17505
Conformer.87	33.667171	8.19978

Conformer.88	33.763939	8.29654
Conformer.89	33.960883	8.49349
Conformer.90	34.073025	8.60563
Conformer.91	34.133318	8.66592
Conformer.92	34.529473	9.06208
Conformer.93	34.580281	9.11289
Conformer.94	34.66889	9.20149
Conformer.95	34.785203	9.31781
Conformer.96	35.05174	9.58434
Conformer.97	35.05174	9.58434
Conformer.98	35.120454	9.65306
Conformer.99	35.340049	9.87265
Conformer.100	35.465196	9.9978

minimized conformers	nmpu#	relative energies (kcal/mol)
Conformer.1	-832.479	0
Conformer.2	-832.478	0.001
Conformer.3	-832.47703	0.00197
Conformer.4	-832.475	0.004
Conformer.5	-832.47693	0.00207

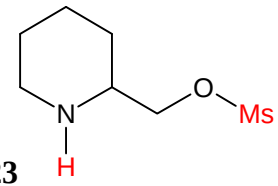
Dih(C17,C16,C15,C14)	Dih(C16,C15,C14,C13)	Dih(C15,C14,C13,C12)	Dih(C14,C13,C12,C11)
(-179.92) -180	(179.89) -180	(179.85) -180	(179.88) 180
(-180.00) 180	(-179.97) 180	(179.99) -180	(-179.99) 179.999
(179.79) 179.845	(175.80) 175.277	(66.05) 66.009	(175.44) 175.289
(179.87) 180	(179.92) 180	(179.75) 179.993	(179.78) 179.996
(-179.99) -180	(179.99) -179.98	(-179.74) -179.84	(-175.85) -175.28

Dih(C13,C12,C11,C10)	Dih(C12,C11,C10,C9)	Dih(C11,C10,C9,C8)	Dih(C10,C9,C8,C7)
(179.83) -180	(179.80) -180	(179.78) 179.975	(-179.91) -178.62
(179.93) -179.99	(179.90) 179.986	(-180.00) -179.91	(-178.80) -178.28
(179.69) 179.832	(179.75) 179.984	(-179.99) 179.994	(179.12) 178.651
(179.39) 179.786	(174.80) 175.397	(61.45) 59.8483	(62.40) 59.3196
(-66.23) -66.001	(-175.74) -175.29	(-179.74) -179.82	(179.74) 178.656

Dih(C9,C8,C7,O1)	Dih(C8,C7,O1,C6)	Dih(C7,O1,C6,C5)	Dih(O1,C6,C5,C4)
(-63.56) -63.623	(179.02) 179.703	(-179.84) 177.693	(-55.48) -58.369
(-63.32) -63.085	(-176.74) 179.488	(179.50) -176.12	(-152.09) -155.99
(64.08) 63.4397	(-179.89) -179.27	(-177.88) 176.927	(-55.16) -58.267
(174.82) 175.611	(179.64) 179.979	(-179.39) 177.418	(-55.26) -58.469
(63.33) 63.5419	(-178.04) 179.886	(-179.85) -177.24	(-153.24) -156.17

Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
(-177.95) -179.77	(53.65) 53.1557	(-53.14) -53.373	(56.63) 57.1253
(-178.06) 179.095	(53.07) 53.487	(-52.71) -52.385	(56.84) 56.3778
(-177.75) -179.74	(53.60) 53.1462	(-53.17) -53.376	(56.69) 57.1297
(-177.95) -179.77	(53.66) 53.161	(-53.16) -53.37	(56.66) 57.1228
(-178.22) 179.115	(53.06) 53.4944	(-52.68) -52.417	(56.84) 56.396

Dih(C2,C1,N1,C18)	Dih(C18,N1,C5,C6)	Dih(N1,C5,C6,O1)
(173.02) 176.517	(-55.32) -58.584	(-177.42) 178.788
(171.62) 175.609	(-55.22) -57.205	(86.44) 82.646
(172.92) 176.523	(-55.27) -58.618	(-177.09) 178.903
(173.02) 176.513	(-55.32) -58.597	(-177.20) 178.707
(171.53) 175.681	(-55.07) -57.324	(85.26) 82.4468



Compound 23

Molecule (-950.28 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	-15.594	0
Conformer.2	-14.214	1.37975
Conformer.3	-13.572	2.022
Conformer.4	-11.381	4.21235
Conformer.5	-11.316	4.27743
Conformer.6	-11.189	4.40471
Conformer.7	-11.162	4.43167
Conformer.8	-10.834	4.75978
Conformer.9	-8.3142	7.27939

minimized conformers		relative energies kcal/mol
Conformer.1	-950.286	0
Conformer.2	-950.283	0.003
Conformer.3	-950.284	0.002
Conformer.4	-950.28	0.006
Conformer.5	-950.28	0.006
Conformer.6	-950.284	0.002
Conformer.7	-950.279	0.007
Conformer.8	-950.279	0.007
Conformer.9	-950.28	0.006

Dih(C7,S1,O1,C6)	Dih(S1,O1,C6,C5)	Dih(O1,C6,C5,C4)
(152.36) 155.656	(73.20) 62.176	(177.16) 177.385
(-176.13) -165.78	(-79.66) -76.574	(-60.21) -57.037
(-177.69) -177.69	(-177.07) -177.07	(-63.44) -63.442
(178.61) 178.001	(177.68) 175.028	(-65.56) -61.991
(176.29) 174.361	(169.98) 166.989	(-61.49) -61.74
(179.93) 163.118	(-177.45) 76.9851	(-65.65) -105.68
(-161.08) -167.11	(-80.94) -77.565	(-53.07) -53.012
(176.55) 179.243	(-111.25) -96.36	(-63.05) -57.357

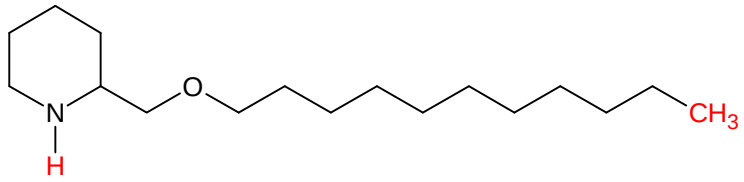
(178.61) 161.176	(177.68) 79.8869	(-65.58) -99.912

Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)
(-175.68) -177.76	(53.05) 52.4185	(-53.15) -52.174
(-172.59) -177.07	(53.60) 52.4285	(-53.91) -52.473
(-177.53)-177.53	(52.38) 52.383	(-52.44) -52.442
(-74.53) -74.429	(-52.39) -52.206	(53.85) 52.1834
(-75.54)-73.984	(-52.49) -51.91	(54.44) 51.9695
(-173.68) -178.25	(53.65) 53.4138	(-53.73) -52.106
(-75.57) -73.957	(-52.81) -52.625	(55.03) 52.5691
(-74.75) -74.033	(-52.27) -52.412	(53.84) 52.192
(-74.54) -73.727	(-52.38) -51.549	(53.85) 51.7651

Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,H2)	Dih(C1,N1,H2,C5)
(56.22) 55.7384	(176.59) -178.25	(124.31) 120.932
(56.18) 55.9175	(177.31) -179.56	(124.98) 121.964
(55.77) 55.7664	(179.76) 179.763	(122.66) 122.659
(-55.46) -54.586	(-172.23) -179.77	(-131.65) -125.23
(-53.51) -54.761	(-173.90) -62.887	(127.50) 122.463
(56.02) 55.3488	(176.35) -179.85	(125.54) 121.82
(-53.35) -54.513	(-75.89) -63.883	(128.37) 22.828
(-55.43) -54.297	(-171.55) -179.43	(-132.33) -125.9
(-55.46) -55.398	(-172.23) -177.86	(-131.63) -125.39

Dih(H2,N1,C5,C6)	Dih(N1,C5,C6,O1)
(-57.32) -60.149	(57.18) 55.092
(-57.77) -59.175	(-179.95) -179.55
(-58.22) -58.224	(173.78) 173.779
(-58.53) -51.197	(170.15) 171.569
(-155.62) -168.32	(171.80) 171.669
(-56.20) -58.859	(174.34) 133.087
(-153.39) -166.89	(-179.58) -179.7

(-59.40) -52.1 (172.81) 176.51
(-58.52) -53.133 (170.13) 135.128



Compound 22

Molecule (-793.00 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	17.5042	0
Conformer.2	17.5373	0.03316
Conformer.3	17.619	0.11485
Conformer.4	17.764	0.25979
Conformer.5	18.1486	0.64442
Conformer.6	18.1582	0.65398
Conformer.7	18.2875	0.78334
Conformer.8	18.3287	0.8245
Conformer.9	18.3288	0.82465
Conformer.10	18.3653	0.8611
Conformer.11	18.4925	0.98828
Conformer.12	18.6892	1.18497
Conformer.13	18.7151	1.21088
Conformer.14	18.8014	1.29723
Conformer.15	18.8129	1.30868
Conformer.16	18.8917	1.38756
Conformer.17	18.9328	1.42857
Conformer.18	39.0939	21.5897
Conformer.19	18.9513	1.44708
Conformer.20	18.9358	1.43158
Conformer.21	18.9807	1.47647
Conformer.22	19.0061	1.50195
Conformer.23	19.07	1.5658
Conformer.24	19.152	1.64784
Conformer.25	19.5415	2.03731
Conformer.26	19.6977	2.19354
Conformer.27	19.738	2.23378

Conformer.28	19.7355	2.23136
Conformer.29	19.7627	2.25853
Conformer.30	19.8291	2.32495
Conformer.31	19.9314	2.42726
Conformer.32	20.0021	2.49794
Conformer.33	20.169	2.66479
Conformer.34	20.2437	2.73955
Conformer.35	20.2864	2.78219
Conformer.36	20.3622	2.85801
Conformer.37	20.3708	2.86664
Conformer.38	20.3959	2.89172
Conformer.39	20.4211	2.91692
Conformer.40	20.5019	2.9977
Conformer.41	20.5394	3.0352
Conformer.42	20.7003	3.19609
Conformer.43	20.7203	3.21608
Conformer.44	20.8007	3.29655
Conformer.45	20.8251	3.32091
Conformer.46	20.8602	3.35601
Conformer.47	21.0125	3.50829
Conformer.48	21.0421	3.5379
Conformer.49	21.0823	3.57814
Conformer.50	21.3581	3.85392
Conformer.51	21.3722	3.868
Conformer.52	21.4028	3.89864
Conformer.53	21.4518	3.94763
Conformer.54	21.3874	3.88317
Conformer.55	21.5361	4.03195
Conformer.56	21.882	4.37777
Conformer.57	21.9144	4.41017
Conformer.58	21.9183	4.41413
Conformer.59	22.0517	4.54756
Conformer.60	22.0916	4.5874
Conformer.61	22.2113	4.70713
Conformer.62	22.6133	5.10907
Conformer.63	22.6313	5.1271
Conformer.64	22.7949	5.29069

Conformer.65	22.898	5.39383
Conformer.66	22.9307	5.42651
Conformer.67	23.2829	5.77876
Conformer.68	23.3617	5.85749
Conformer.69	23.3886	5.88438
Conformer.70	23.459	5.95482
Conformer.71	23.4635	5.95933
Conformer.72	23.5229	6.01875
Conformer.73	23.5775	6.07336
Conformer.74	23.6562	6.15205
Conformer.75	23.9021	6.39791
Conformer.76	24.0368	6.53259
Conformer.77	24.1627	6.65856
Conformer.78	24.1627	6.65856
Conformer.79	24.6672	7.16304
Conformer.80	24.7268	7.22266
Conformer.81	24.7826	7.27841
Conformer.82	24.8439	7.33972
Conformer.83	24.8442	7.34001
Conformer.84	24.8602	7.35603
Conformer.85	25.0723	7.56813
Conformer.86	25.3606	7.85638
Conformer.87	25.3712	7.867
Conformer.88	25.7767	8.2725
Conformer.89	25.8797	8.37551
Conformer.90	25.9326	8.42844
Conformer.91	26.3208	8.81664
Conformer.92	26.3963	8.89214
Conformer.93	26.7663	9.26206
Conformer.94	26.8089	9.30476
Conformer.95	26.8301	9.32593
Conformer.96	26.8692	9.36498
Conformer.97	26.8904	9.38626
Conformer.98	27.0051	9.50089
Conformer.99	27.0081	9.50395
Conformer.100	27.1492	9.64506

minimized conformers		relative energies kcal/mol
Conformer.1	-793.4567	0.0002
Conformer.2	-793.4569	0
Conformer.3	-793.4554	0.0015
Conformer.4	-793.4550	0.0019
Conformer.5	-793.4552	0.0017
Conformer.6	-793.4527	0.0042

Dih(C17,C16,C15,C14)	Dih(C16,C15,C14,C13)	Dih(C15,C14,C13,C12)	Dih(C14,C13,C12,C11
(-179.89) 180	(179.82) -180	(-179.78) -180	(179.73) 18
(-179.95) -65.555	(-179.52) -177.44	(-179.98) 179.079	(-179.29) -177.2
(-179.98) -180	(-179.91) 180	(-179.98) -180	(-179.88) 18
(179.97) 64.963	(179.99) 172.969	(179.95) 178.408	(179.95) -178.2
(65.61) 179.999	(175.85) -180	(179.80) 179.998	(179.64) -179.9
(-179.03) 175.670	(-175.53) 60.470	(-175.18) 55.928	(-56.86) 60.397

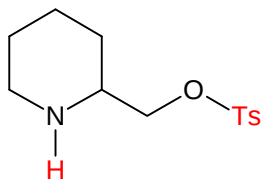
Dih(C13,C12,C11,C10)	Dih(C12,C11,C10,C9)	Dih(C11,C10,C9,C8)	Dih(C10,C9,C8,C7)
(-179.75) -180	(179.81) 180	(-179.78) -180	(179.94) 179.996
(179.93) -58.442	(-179.49) -60.79	(179.78) -178.87	(-179.54) -62.14
(179.98) -180	(179.42) 179.997	(174.89) 179.992	(61.68) -178.65
(179.83) -58.268	(179.65) -61.925	(175.05) 177.862	(66.19) -64.125
(-179.86) 179.962	(179.84) -179.63	(-179.95) -175.57	(178.71) -61.332
(-57.67) 175.702	(-177.93) 179.827	(-179.59) 179.997	(60.11) 179.996

Dih(C9,C8,C7,O1)	Dih(C8,C7,O1,C6)	Dih(C7,O1,C6,C5)	Dih(O1,C6,C5,C4)
(-179.79) -179.97	(-179.99) -179.83	(176.83) -178.27	(177.17) 64.5615

(-63.61) -52.383	(178.84) 174.773	(176.24) -178.11	(177.04) 172.367
(58.30) -63.49	(179.13) 179.349	(177.20) -177.82	(176.94) 64.2793
(175.30) -52.66	(179.51) 173.68	(176.90) -178.87	(177.16) 172.265
(63.63) -55.55	(179.07) 178.365	(177.49) -176.41	(176.48) 64.1922
(55.86) 179.973	(-177.52) 179.59	(178.31) 177.266	(177.30) 173.487

Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
(176.41) 177.524	(-52.76) -52.348	(52.59) 52.4729	(-55.87) -55.995
(176.32) 178.756	(-52.74) -52	(52.59) 51.0829	(-55.87) -55.089
(176.43) 177.523	(-52.78) -52.337	(52.61) 52.479	(-55.89) -56.001
(176.39) 178.591	(-52.76) -52.112	(52.59) 51.3272	(-55.87) -55.292
(176.44) 177.5	(-52.76) -52.327	(52.57) 52.4815	(-55.86) -56.008
(176.91) 178.162	(-52.83) -52.194	(52.48) 51.4144	(-55.79) -55.29

Dih(C2,C1,N1,C5)	Dih(C1,N1,H4,C5)	Dih(H4,N1,C5,C6)	Dih(N1,C5,C6,O1)
(61.82) 58.9723	(-125.24) -121.94	(52.72) 58.9489	(-62.15) -172.65
(-175.34) 60.2129	(-125.30) -121.32	(52.75) 55.6065	(-62.33) -65.412
(-175.38) 58.961	(-125.22) -121.94	(52.85) 58.9693	(-62.43) -172.92
(-175.38) 60.2397	(-125.25) -121.36	(52.71) 55.7622	(-62.18) -65.537
(61.86) 58.961	(-125.31) -121.94	(52.71) 59.0312	(-62.89) -173.02
(61.81) 60.1791	(-124.84) -121.55	(52.97) 56.0397	(-61.93) -64.586



Compound 24

Molecule (-1179.818 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	33.84482	0
Conformer.2	33.984759	0.13994
Conformer.3	34.853729	1.00891
Conformer.4	36.236948	2.39213
Conformer.5	36.781721	2.9369
Conformer.6	36.850053	3.00523
Conformer.7	37.002111	3.15729
Conformer.8	37.016452	3.17163
Conformer.9	37.388272	3.54345

minimized conformers		relative energies kcal/mol
Conformer.1	-1179.8173	0.000000
Conformer.2	-1179.8156	0.001700
Conformer.3	-1179.8157	0.001600
Conformer.4	-1179.8123	0.005000
Conformer.5	-1179.8141	0.003200
Conformer.6	-1179.814874	0.002426
Conformer.7	-1179.814871	0.002429
Conformer.8	-1179.814875	0.002425
Conformer.9	-1179.8135	0.003800

Dih(C11,C10,C9,C8)	Dih(C10,C9,C8,C7)	Dih(C9,C8,C7,S1)	Dih(C8,C7,S1,O1)
(179.93) -178.56	(-0.13) 0.41697	(-178.14) 179.322	(-120.00) -130.23
(-178.79) -178.57	(0.04) 0.45735	(179.96) 179.438	(-89.81) -127.98

(-179.15) -178.57	(0.12) 0.46167	(179.94) 179.369	(-87.00) -53.822
(179.72) -178.43	(-0.05) 0.58116	(-178.21) 179.69	(-122.69) -124.04
(179.18) 178.376	(0.41) -0.3722	(179.62) 178.071	(-75.00) -60.508
(179.77) -178.71	(0.08) 0.49115	(180.00) 178.691	(-106.34) -126.12
(179.26) 178.36	(0.13) -0.663	(179.99) 178.565	(-106.04) -133.78
(179.79) -178.65	(0.08) 0.34743	(179.93) 178.472	(-106.47) -133.85
(179.60) -178.71	(0.42) 0.51932	(-179.63) 177.883	(-68.05) -46.038

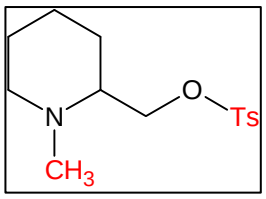
Dih(C7,S1,O1,C6)	Dih(S1,O1,C6,C5)	Dih(O1,C6,C5,C4)	Dih(C6,C5,C4,C3)
(-153.26) -154.18	(116.26) 108.068	(176.99) 175.316	(99.48) 87.3561
(172.74) -162.43	(135.71) 110.636	(173.16) 167.923	(66.26) 74.2057
(174.17) 148.774	(169.92) -94.988	(176.89) 178.767	(66.37) 71.7505
(85.29) 110.848	(-100.22) -75.608	(-173.14) -176.78	(98.36)87.4869
(-80.95) -83.714	(178.97) 157.553	(178.01) 176.005	(66.54) 69.6307
(81.25) 74.6595	(174.49) 106.726	(179.37) 164.31	(66.38) 70.9469
(81.63) 91.7394	(174.02) -167.68	(179.50) 178.047	(66.39)70.3705
(80.95) 92.0843	(174.47)-167.74	(179.21) 178.063	(66.38) 70.3765
(-82.09) -83.517	(172.00) 152.648	(174.95) 170.293	(100.88) 89.9593

Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C5)
(60.81) 54.2835	(-35.14) -12.48	(-24.55) -44.848	(63.44) 61.9501
(36.04) 40.0131	(19.79) 13.3904	(-57.59) -59.146	(35.35) 47.2608
(35.54) 36.6434	(20.23) 17.1521	(-57.11) -59.615	(34.14) 43.1026
(60.77) 54.1427	(-34.78) -13.505	(-24.71) -43.982	(63.01) 62.5103
(34.96) 33.8248	(20.80) 20.7601	(-56.84) -58.746	(33.13) 36.7414
(34.61) 36.9386	(21.18) 17.8729	(-57.01) -59.445	(32.93) 41.2645
(34.52) 34.0489	(21.27) 20.3718	(-57.01) -58.968	(32.83) 37.6015
(34.50) 34.0492	(21.21) 20.3713	(-57.00) -58.972	(32.87) 37.6087
55.9825	-17.412	-41.542	64.6617

Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,O1)	Dih(O1,S1,O3,O2)

(-159.33) -144.44	(-57.70) -57.062	(-123.83) -125.38
(-102.16) -118.58	(-62.84) -64.31	(-123.76) -125.01
(-101.10) -113.51	(-59.17) -53.925	(-124.14)-124.86
(-157.90) -145.5	(-48.17) -49.72	(-120.86) -125
(-100.30) -106.4	(-58.10) -57.344	(-123.10) -125.97
(-99.88) -110.8	(-56.77) -68.847	(-121.22)-125.53
(-99.79) -107.78	(-56.65) -54.7	(-121.22)-125.58
(-99.84) -107.79	(-56.92) -54.681	(-121.23)-125.57
(-160.81) -149.64	(-59.71) -63.226	(-123.34) -125.61

Compound 19



Molecule (-1218.853 kcal/mol)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	35.026267	0
Conformer.2	35.525023	0.49876
Conformer.3	35.589505	0.56324
Conformer.4	35.708324	0.68206
Conformer.5	36.511628	1.48536
Conformer.6	37.382635	2.35637
Conformer.7	38.14402	3.11775
Conformer.8	38.340278	3.31401
Conformer.9	39.068518	4.04225
Conformer.10	39.436262	4.40999
Conformer.11	41.001197	5.97493

minimized conformers		relative energies kcal/mol
Conformer.1	-1218.8526	0.0012
Conformer.2	-1218.8538	0
Conformer.3	-1218.8528	0.001

Conformer.4	-1218.8531	0.0007
Conformer.5	-1218.8526	0.0012
Conformer.6	-1218.8508	0.003
Conformer.7	-1218.8495	0.0043
Conformer.8	-1218.8497	0.0041
Conformer.9	-1218.8503	0.0035
Conformer.10	-1218.8492	0.0046
Conformer.11	-1218.8484	0.0054

Dih(C14,C9,C13,C10)	Dih(C9,C13,C10,C8)	Dih(C13,C10,C8,S1)
(178.83) 178.553	(-0.07) -0.4061	-179.18
(178.89) -178.44	(-0.07) 0.62289	-179.21
(-178.96) -178.45	(-0.23) 0.51177	-178.79
(-179.44) 178.703	(-0.35) -0.4704	-178.69
(-179.61) 178.58	(-0.12) -0.463	-179.33
(178.94) 178.591	(-0.09) -0.4473	-179.27
(179.56) 178.602	(-0.11) -0.5861	-178.39
(-179.29) 178.592	(-0.40) -0.4809	-178.87
(-178.4	(-0.10) 0.53051	-179.25
178.556	(-0.40) -0.3827	-179.13

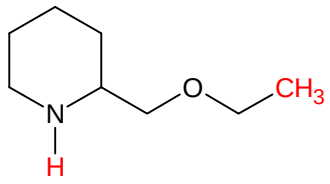
Dih(C10,C8,S1,O2)	Dih(C10,C8,S1,O3)	Dih(C8,S1,O1,C7)	Dih(S1,O1,C7,C3)
17.1379	-114.52	171.231	81.6671
18.335	-113.08	-151.34	-70.736
-59.471	169.057	83.0541	-166.84
11.6644	-119.79	-86.049	171.719
13.6299	-118.34	-176.8	-168.78
14.9713	-116.75	167.639	79.5521
-54.955	173.533	82.0773	-163.35
11.4592	-119.9	-83.754	172.531
-56.576	172.249	79.6457	93.9682
18.9802	-112.64	-159.73	-78.494

Dih(O1,C7,C3,C5)	Dih(C7,C3,C5,C1)	Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)
51.7098	179.209	-53.214	53.4149

159.748	-179.91	-53.694	52.7569
56.8108	179.348	-53.089	53.3223
58.674	179.746	-53.218	53.4305
60.6446	74.0954	52.001	-51.974
52.6615	74.035	52.6089	-52.522
59.6409	73.8132	52.3696	-52.18
62.3444	74.2734	51.7014	-51.864
55.9177	74.1447	52.3138	-52.431
97.6238	73.6078	51.2887	-51.439

Dih(C1,C6,C2,N1)	Dih(C2,N1,C4,C3)	Dih(C4,N1,C3,C7)	Dih(N1,C3,C7,O1)
-57.069	-123.46	58.8743	174.36
-56.493	-123.54	58.9188	-79.19
-57.013	-123.86	58.4348	179.446
-56.938	-124.05	58.2647	-178.37
52.8896	-127.49	157.405	-172.43
52.7804	-127.54	156.566	179.646
52.7643	-127.64	157.191	-173.59
53.0391	-127.28	157.484	-170.63
52.9423	-127.53	156.593	-177.18
53.6755	-127.93	157.974	-136.76

Dih(O2,S1,O1,C7)	Dih(O3,S1,O1,C7)
-74.909	58.0283
-37.263	95.765
-164.14	-31.375
28.1407	161.274
-62.699	70.1784
-78.753	54.6327
-165.24	-32.176
30.7116	163.459
-167.59	-34.989
-45.697	87.3411



Compound 21

Molecule (-442.141 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	20.4797	0
Conformer.2	21.5686	1.08886
Conformer.3	21.8397	1.35998
Conformer.4	21.9821	1.50243
Conformer.5	22.0609	1.58122
Conformer.6	22.2141	1.73437
Conformer.7	23.1504	2.67069
Conformer.8	23.502	3.02228
Conformer.9	23.6394	3.15976
Conformer.10	23.7689	3.28924
Conformer.11	25.0749	4.59517
Conformer.12	26.1071	5.62745
Conformer.13	26.2066	5.72693
Conformer.14	27.2514	6.77171
Conformer.15	27.8806	7.40093
Conformer.16	27.9148	7.43509

minimized conformers (2ep#)		relative energy (kcal/mol)
Conf1:	-442.1409	0
Conf2:	-442.1385	0.0024
Conf4:	-442.1383289	0.002571
Conf5:	-442.1383187	0.002581
Conf12:	-442.1409	0
Conf16:	-442.1383187	0.002581

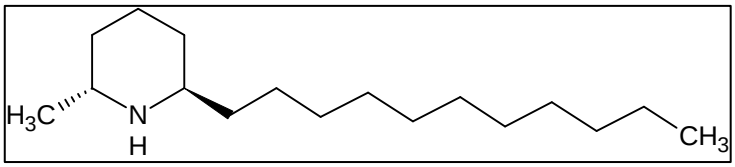
Dih(C8,C7,O1,C6)	Dih(C7,O1,C6,C5)	Dih(O1,C6,C5,C4)
(179.54) -179.7	(-179.18) -178.78	(-58.66) -60.14
(-176.99) -177.87	(-83.49) -79.778	(-55.51) -55.827
-79.24	-177.44	-178.9
(-51.84) -80.328	(-174.34) -177.16	(-58.70) -60.51
(78.87) 81.0843	(176.25) 179.378	(-58.52) -60.041
179.982	179.866	-62.04
-85.76	-84.712	-57.76
-176.32	-77.508	-55.027
-82.457	179.194	-62.215
78.8575	176.593	-62.102
-85.749	-84.205	-57.767
(179.54) 167.161	(-179.18) 73.3211	(-58.66) -97.141
171.076	74.3644	-101.85
-72.274	110.728	-173.51
70.7399	71.7853	-105.45
(78.87) 67.3078	(176.25) 69.7745	(-58.52) -100.96

Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)
(-177.71) -178.13	(52.79) 51.9223	(-52.05) -51.747
(-176.79) -177.62	(52.92) 51.9916	(-52.24) -52.02
-75.187	-51.686	52.5965
(-177.56) -178.12	(52.89) 51.9263	(-52.10) -51.754
(-177.62) -178.14	(52.88) 51.9277	(-52.10) -51.748
-74.483	-52.13	52.1916
-177.68	51.9991	-51.987
-74.551	-52.545	52.5265
-74.388	-52.188	52.191
(-177.71) -74.478	(52.79) -52.125	(-52.05) 52.1737
-74.615	-52.244	52.3632
-178.55	53.0857	-51.393
-73.856	-51.484	51.6641

-177.77	52.6681	-52.469
-73.91	-51.635	51.8094
(-177.62) -178.65	(52.88) 53.1587	(-52.10) -51.404

Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,O1)
(53.07) 55.8466	(-54.75)-59.526	(-178.82) -177.71	(175.59) 176.8
(52.98) 55.8468	(-54.27) -59.047	(-179.96) -178.51	(179.10) -178.96
-55.321	56.6541	72.5972	54.3773
(52.98) 55.8499	(-54.57) -59.523	(-179.02) -177.77	(175.61) 176.449
(52.98) 55.8475	(-54.58) -59.537	(-178.88) -177.69	(175.72) 176.901
-54.729	56.9729	71.8718	171.522
55.8367	-59.105	-178.47	179.154
-54.6	56.3139	72.6653	178.263
-54.671	56.9088	71.794	171.398
-54.728	57.007	71.8432	171.47
-54.761	56.674	72.3612	175.62
(53.07) 55.1001	(-54.75) -60.27	(-178.82) -177.2	(175.59) 141.716
-55.479	59.106	69.7729	133.171
55.5646	-58.342	179.383	63.8594
-55.464	58.8926	69.895	129.543
(52.98) 55.0621	(-54.58) -60.231	(-178.88) -177.35	(175.72) 137.964

Compound 40



Molecule (-718.6098 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	-7.40318	0
Conformer.2	-7.19759	0.205593
Conformer.3	-6.87719	0.525995
Conformer.4	-6.63668	0.766501
Conformer.5	-6.45427	0.948916

Conformer.6	-6.01898	1.384206
Conformer.7	-6.00831	1.394874
Conformer.8	-5.98711	1.416076
Conformer.9	-5.84987	1.553318
Conformer.10	-5.75415	1.649031
Conformer.11	-5.28801	2.115177
Conformer.12	-5.28729	2.115894
Conformer.13	-5.15516	2.248022
Conformer.14	-5.15244	2.25074
Conformer.15	-5.00145	2.40173
Conformer.16	-4.99008	2.413107
Conformer.17	-4.97662	2.426559
Conformer.18	-4.83741	2.565769
Conformer.19	-4.79254	2.610641
Conformer.20	-4.75036	2.65282
Conformer.21	-4.7663	2.636884
Conformer.22	-4.62711	2.776075
Conformer.23	-4.61052	2.792662
Conformer.24	-4.5262	2.87698
Conformer.25	-4.52937	2.873815
Conformer.26	-4.52936	2.873827
Conformer.27	-4.4653	2.937879
Conformer.28	-4.46369	2.939489
Conformer.29	-4.4614	2.941786
Conformer.30	-4.4442	2.958987
Conformer.31	-4.2652	3.137979
Conformer.32	-4.23776	3.165427
Conformer.33	-4.10461	3.298578
Conformer.34	-4.07496	3.328222
Conformer.35	-4.03106	3.37212
Conformer.36	-3.90977	3.493418
Conformer.37	-3.83839	3.564793
Conformer.38	-3.82958	3.573605
Conformer.39	-3.72441	3.67877
Conformer.40	-3.69306	3.710127
Conformer.41	-3.61673	3.786455
Conformer.42	-3.56908	3.834109
Conformer.43	-3.31243	4.090755
Conformer.44	-3.30723	4.095953
Conformer.45	-3.25661	4.146575
Conformer.46	-3.17118	4.232008
Conformer.47	-3.16327	4.23991
Conformer.48	-3.07593	4.327254

Conformer.49	-2.9335	4.469688
Conformer.50	-2.78345	4.619733
Conformer.51	-2.64835	4.754831
Conformer.52	-2.54504	4.858141
Conformer.53	-2.47247	4.930717
Conformer.54	-2.44407	4.959111
Conformer.55	-2.37928	5.023906
Conformer.56	-2.36481	5.038371
Conformer.57	-2.36243	5.04075
Conformer.58	-2.23586	5.167323
Conformer.59	-2.1787	5.224483
Conformer.60	-2.0439	5.359281
Conformer.61	-1.92748	5.475704
Conformer.62	-1.89276	5.51042
Conformer.63	-1.85975	5.543437
Conformer.64	-1.82011	5.58307
Conformer.65	-1.73316	5.670025
Conformer.66	-1.68722	5.715967
Conformer.67	-1.68606	5.717127
Conformer.68	-1.68117	5.722016
Conformer.69	-1.59549	5.80769
Conformer.70	-1.53291	5.870275
Conformer.71	-1.48961	5.913578
Conformer.72	-1.3795	6.023681
Conformer.73	-1.37568	6.027502
Conformer.74	-1.22414	6.179043
Conformer.75	-1.11044	6.292749
Conformer.76	-1.07622	6.326964
Conformer.77	-0.93369	6.469492
Conformer.78	-0.86757	6.535611
Conformer.79	-0.83606	6.56712
Conformer.80	-0.74189	6.661293
Conformer.81	-0.71738	6.685801
Conformer.82	-0.70499	6.698196
Conformer.83	-0.68828	6.714905
Conformer.84	-0.68768	6.715505
Conformer.85	-0.43165	6.97153
Conformer.86	-0.40724	6.995942
Conformer.87	-0.17006	7.233124
Conformer.88	0.001674	7.404858
Conformer.89	0.172247	7.575431
Conformer.90	0.480938	7.884122
Conformer.91	0.577817	7.981001

Conformer.92	0.892778	8.295962
Conformer.93	0.912937	8.316121
Conformer.94	0.936647	8.339831
Conformer.95	0.973538	8.376722
Conformer.96	1.329661	8.732845
Conformer.97	1.534143	8.937327
Conformer.98	1.913616	9.3168
Conformer.99	2.18355	9.586734
Conformer.100	2.515904	9.919088

minimized conformers I21#		relative energies kcal/mol
Conformer.1	-718.6100	0
Conformer.2	-718.6098	0.0002
Conformer.3	-718.6083	0.0017
Conformer.4	-718.6084	0.0016
Conformer.5	-718.6079	0.0021

Dih(C17,C16,C15,C14)	Dih(C16,C15,C14,C13)	Dih(C15,C14,C13,C12)
(179.99) -180	(179.97) -180	(-180.00) -180
(-179.95) -180	(179.87) -180	(-179.89) 180
(-179.79) 180	(179.99) 180	(-179.59) -180
(179.97) -180	(-179.95) -180	(179.98) -180
(179.94) 180	(179.90) -180	(179.90) -180

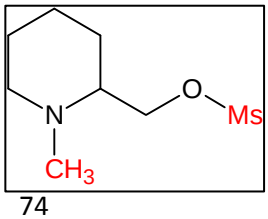
Dih(C13,C12,C11,C10)	Dih(C12,C11,C10,C9)	Dih(C11,C10,C9,C8)
(-179.98) -180	(179.85) -179.996	(-179.78) -179.97
(-179.87) 179.9996	(179.79) 179.9957	(179.93) 179.9701
(-179.54) -179.992	(-179.92) -179.993	(-179.21) -179.722
(-179.90) -179.98	(-179.67) -179.837	(-175.77) -175.41
(179.95) 179.9904	(-179.84) -179.794	(-175.23) -175.893

Dih(C9,C8,C7,C6)	Dih(C8,C7,C6,C5)	Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)
(-174.42) -174.84	(173.28) 173.009	(177.01) 177.943	(-53.09) -52.9597
(174.30) 174.431	(64.83) 62.9733	(175.45) 175.399	(-53.01) -52.4335
(-60.70) -58.8151	(177.89) 178.225	(176.85) 177.917	(-53.19) -52.9561
(-169.73) -170.16	(173.73) 173.535	(176.93) 177.906	(-53.13) -52.9472
(-58.15) -55.0683	(178.20) 177.564	(176.85) 177.888	(-53.19) -52.948

Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C1,C2,N1,C6)
(53.08) 52.761	(-176.51) -176.778	(61.06) 59.36324
(53.09) 52.73209	(-176.32) -176.982	(61.27) 59.75184
(53.13) 52.72828	(-176.54) -176.756	(61.08) 59.41705
(53.14) 52.76065	(-176.50) -176.772	(61.00) 59.35092
(53.15) 52.70127	(-176.53) -176.736	(61.04) 59.44176

Dih(C2,N1,C6,C7)	Dih(N1,C6,C7,C8)	Dih(H4,N1,C6,C7)
(177.22) 179.513	(-66.03) -65.091	(54.22) 58.14951
(175.70) 178.047	(-174.65) -175.26	(52.07) 56.22623
(177.61) 179.534	(-61.72) -59.974	(54.43) 58.26362
(177.25) 179.491	(-65.57) -64.553	(54.14) 58.10206
(177.62) 179.459	(-61.38) -60.659	(54.44) 58.12216

Compound 18



Molecule (-989.31 kcal/mol)		E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer1		-6.91829799	0
	2	-6.13426299	0.784034999
	3	-6.12400699	0.794290999
	4	-6.09944799	0.818849999
	5	-3.630087	3.288211
	6	-3.510946	3.407352
	7	-3.253862	3.664436
	8	-0.937383999	5.98091399

minimized conformers			relative energies kcal/mol
Conformer1		-989.3080	0.0006
	2	-989.3077	0.0009
	3	-989.3086	0
	4	-989.3076	0.001
	5	-989.3057	0.0029
	6	-989.3047	0.0039
	7	-989.3031	0.0055
	8	-989.3038	0.0048

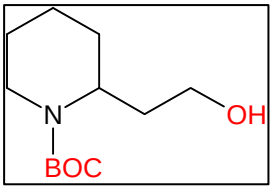
Dih(C8,S1,O1,C7)	Dih(S1,O1,C7,C3)	Dih(O1,C7,C3,C5)	Dih(C7,C3,C5,C1)
(156.62) 169.154	(83.84) 79.0462	(51.74) 52.5623	(175.04) 179.349
(-178.30) 176.65	(-100.51) -94.14	(155.20) 157.912	(176.66) -179.68
(-179.65) 177.929	(175.27) 178.786	(57.19) 57.5384	(176.30) 179.839

(-152.52) -154.39	(-81.71) -72.407	(157.22) 159.928	(176.80) -179.85
(-177.40) -174.84	(-172.10) -167.63	(61.84) 61.4116	(74.58) 74.1454
(159.81) 166.868	(80.47) 77.7581	(53.79) 53.1283	(74.58) 74.0807
(177.00) 160.951	(-99.75) -94.071	(173.58) 177.608	(76.07) 74.7168
(-128.08) -159.27	(-118.30) -79.103	(63.76) 96.9811	(74.22) 73.6161

Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)	Dih(C1,C6,C2,N1)	Dih(C6,C2,N1,C4)
(-53.82) -53.26	(53.88) 53.368	(-56.88)-57.034	(-174.47)-176.7
(-53.26) -53.623	(53.20) 52.7131	(-56.93) -56.47	(-172.55) -175.53
(-53.82) -53.172	(53.56) 53.3018	(-56.73) -56.889	(-173.46) -176.07
(-53.18) -53.674	(53.13) 52.7313	(-57.00) -56.518	(-172.51) -175.69
(52.08) 51.8949	(-53.81) -51.901	(54.72) 52.9335	(80.27) 74.9416
(52.37) 52.5629	(-54.38) -52.503	(54.72) 52.8115	(81.49) 75.5787
(52.13) 51.7513	(-53.71) -51.945	(54.65) 53.1233	(80.74) 74.8967
(52.23) 51.2808	(-53.90) -51.44	(54.68) 53.6857	(80.20) 73.7357

Dih(C2,N1,C4,C3)	Dih(C4,N1,C3,C7)	Dih(N1,C3,C7,O1)
(-126.26) -123.39	(58.04) 58.8504	(173.05) 175.136
(-126.84) -123.69	(57.72) 58.1006	(-84.03) -80.726
(-126.64) -124.02	(56.32) 57.9623	(178.72) -179.61
(-126.63) -123.43	(58.04) 58.9293	(-82.12) -79.009
(-132.49) -127.46	(149.22) 157.505	(-171.21) -171.66
(-132.92) -127.59	(147.72) 156.556	(-179.43) -179.92
(-133.14) -127.53	(150.12) 157.911	(-59.66) -55.684
(-132.17) -127.9	(149.16) 157.958	(-169.25) -137.4

Compound 26



Molecule (-	E	Rel. E

746.8673001 au)	gas(kcal/mol)	gas(kcal/mol)
Conformer.1	-32.408114	0
Conformer.2	-32.322455	0.085659
Conformer.3	-32.238377	0.169737
Conformer.4	-32.072288	0.335826
Conformer.5	-32.040016	0.368098
Conformer.6	-31.752725	0.655388999
Conformer.7	-31.302119	1.105995
Conformer.8	-30.10914	2.298974

Conformation	Energies	Relative Energies
Conformer.1	-746.8696878	0.001499
Conformer.2	-746.8711864	0
Conformer.3	-746.8694855	0.001701
Conformer.4	-746.8703885	0.000798
Conformer.5	-746.8692667	0.00192
Conformer.6	-746.8705729	0.000614
Conformer.7	-746.8701758	0.001011
Conformer.8	-746.8689553	0.002231

Dih(O3,C7,C6,C5)		Dih(C7,C6,C5,C4)		Dih(C6,C5,C4,C3)		Dih(C5,C4,C3,C2)	
(177.68)	177.604	(69.26)	66.3876	(65.55)	67.8358	(35.82)	34.38633

(53.89) 55.5405	(66.87) 61.2365	(65.55) 67.4263	(35.82) 35.39109
(174.49) 176.7658	(67.90) 65.1479	(65.18) 67.6733	(36.17) 34.38177
(55.28) 53.5108	(60.27) 55.3442	(64.74) 66.8754	(36.56) 35.78852
(171.58) 173.7123	(68.00) 62.0462	(65.70) 67.4884	(36.21) 35.06821
(-74.79) -76.3629	(69.01) 68.72115	(64.78) 66.8230	(36.22) 34.64839
(-72.55) -78.8976	(68.78) 65.0676	(65.73) 66.9546	(35.86) 35.09325
(74.75) 60.5518	(80.50) 58.1691	(67.320 67.1205	(33.01) 35.39412

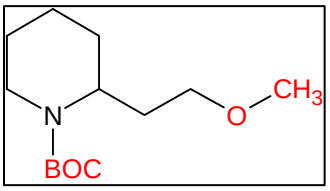
Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C8)	Dih(C1,N1,C8,O2)
(22.22) 20.41076	(-58.21) -55.69502	(-154.54) -153.316	(-178.06) -178.215
(22.08) 19.39066	(-58.16) -55.53078	(-155.37) -153.518	(-178.37) -177.654
(21.86) 20.46983	(-58.02) -55.46960	(-153.68) -153.216	(-177.59) -178.209
(21.31) 19.18467	(-57.66) -55.28706	(-155.57) -153.599	(-177.45) -177.503
(21.73) 19.77305	(-58.07) -55.40936	(-153.94) -153.253	(-177.51) -177.746
(21.92) 20.60453	(-57.98) -55.48513	(-154.35) -154.405	(-177.85) -178.202
(22.10) 20.05798	(-58.19) -55.46515	(-154.74) -154.395	(-177.75) -177.689
(24.81) 19.48870	(-59.15) -55.09597	(-152.48) -153.649	(-177.50) -177.499

Dih(N1,C8,O2,C9)	Dih(O1,C8,N1,C5)	Dih(C8,O2,C9,C11)	Dih(O2,C8,N1,C5)
(179.12) -179.535	(172.96) 174.843	(-179.48) 179.817	(-7.44) -5.2434
(178.01) 179.929	(171.72) 174.430	(-179.36) -179.947	(-8.87) -5.7762
(-178.98) -178.637	(174.10) 175.361	(179.98) 179.429	(-6.10) -4.5103
(179.33) -179.675	(172.47) 174.867	(-179.33) 179.892	(-8.01) -5.2268
(-179.64) -178.965	(173.60) 175.199	(-179.88) 179.606	(-6.70) -4.8304
(-179.64) -179.534	(173.57) 174.939	(-179.50) 179.834	(-6.79) -5.1572
(-167.78) -179.735	(172.88) 174.768	(-179.38) 179.934	(-7.57) -5.3959
(-177.07) -178.979	(176.22) 175.293	(-180.00) 179.578	(-3.93) -4.6281

Dih(N1,C5,C6,C7)
(-167.71) -169.129
(-170.12) -174.505
(-169.20) -170.394
(-168.87) 179.404
(-167.87) -173.582
(-167.87) -166.800

(-167.78) -170.467
(-156.11) -177.603

Compound 28



Molecule (-785.8936451)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	-27.828472	0
Conformer.2	-27.734232	0.09424
Conformer.3	-27.402481	0.425990999
Conformer.4	-27.207212	0.621259999
Conformer.5	-26.5566	1.271872
Conformer.6	-26.316522	1.51195
Conformer.7	-25.876542	1.95193
Conformer.8	-24.500545	3.327927
Conformer.9	-23.251821	4.57665099
Conformer.10	-22.768481	5.05999099

Conformation	Energies	Relative Energies
Conformer.1	-785.8995318	0.000155
Conformer.2	-785.8985868	0.0011
Conformer.3	-785.899687	0
Conformer.4	-785.8969584	0.002729
Conformer.5	-785.8959585	0.003728
Conformer.6	-785.895824	0.003863
Conformer.7	-785.8967075	0.002979
Conformer.8	-785.8962244	0.003463
Conformer.9	-785.8936438	0.006043
Conformer.10	-785.8995327	0.000154

Dih(C8,O3,C7,C6)	Dih(O3,C7,C6,C5)	Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)
(178.61) 178.8040	(54.99) 53.37347	(59.91) 55.48499	(64.78) 66.88943
	(174.45)		
(179.91) -178.9408	176.53958	(68.26) 65.22911	(65.26) 67.62731
(-178.50) -179.3905	(-75.41) -76.76971	(68.49) 67.77731	(64.80) 66.67363
(77.57) 77.2599	(49.41) 48.51567	(54.66) 55.27922	(64.47) 66.87495
	(179.51) -		
(-81.10) -82.2642	179.8247	(69.76) 68.43735	(65.47) 68.04627
	(167.20)		
(77.97) 76.73390	169.29478	(66.98) 61.75861	(65.46) 67.44791
(-86.39) -83.70542	(-74.95) -73.52789	(68.51) 68.84981	(66.01) 66.97765
(-179.17) -	(179.55) -		(114.07)
178.69342	179.86074	(70.00) 72.94032	103.52299
	(-175.13) -		(114.51)
(-78.76) -80.45709	175.32051	(70.45) 74.52754	102.96873
(178.65) -80.93308	(55.22) 99.19706	(60.22) 62.83965	(64.77) 67.16638

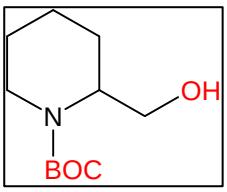
Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
(36.51) 35.77128	(21.38) 19.18987	(-57.69) -55.27724
(35.99) 34.43636	(22.08) 20.42776	(-58.12) -55.46878
(36.25) 34.79514	(21.88) 20.48295	(-57.97) -55.38186
(36.75) 35.67306	(21.19) 19.29067	(-57.50) -55.37806
(35.73) 34.13128	(22.41) 20.69668	(-58.27) -55.86412
(36.60) 35.17256	(21.32) 19.65458	(-57.90) -55.32268
(35.50) 34.54774	(22.41) 20.68875	(-58.28) -55.66987
(-43.33) -29.02882	(66.95) 60.47841	(-31.57) -38.35109
(-43.67) -27.89967	(67.10) 60.26107	(-31.49) -39.76940
(36.62) 35.15327	(21.26) 19.81902	(-57.65) -55.45551

Dih(C2,C1,N1,C9)	Dih(C1,N1,C9,O2)	Dih(N1,C9,O2,C10)	Dih(C9,O2,C10,C12)

(-155.76) -153.580	(-177.50) -177.520	(179.19) -179.634	(-179.36) 179.875
(-154.14) -153.170	(-177.76) -178.233	(-179.57) -178.607	(-179.98) 179.419
(-154.39) -154.496	(-177.86) -178.187	(-179.97) -179.504	(-179.50) 179.821
(-156.83) -154.321	(-177.71) -177.612	(178.12) 179.224	(-179.41) 179.909
(-154.38) -152.640	(-178.13) -178.614	(179.42) -178.779	(-179.62) 179.454
(-153.80) -153.058	(-177.42) -177.814	(-179.50) -178.802	(-179.94) 179.531
(-154.85) -154.425	(-177.77) -177.966	(179.26) -179.682	(-61.86) -63.003
(165.15) 179.283	(174.51) 171.503	(178.35) -178.639	(-62.01) -63.309
(165.06) -179.228	(174.36) 171.298	(177.91) -178.878	(-61.67) -63.112
(-155.62) -152.865	(-177.37) -177.876	(179.49) -177.973	(-61.77) -63.591

Dih(O1,C9,N1,C5)	Dih(C9,N1,C5,C6)	Dih(N1,C5,C6,C7)
(172.27) 174.886	(86.64) 82.429	(-177.32) 179.569
(173.60) 175.371	(85.00) 81.826	(-168.77) -170.325
(173.51) 174.965	(84.83) 82.578	(-168.39) -167.742
(171.34) 173.946	(87.87) 83.252	(177.54) 179.417
(173.23) 175.187	(85.29) 81.298	(-167.22) -167.019
(173.96) 175.340	(84.56) 81.738	(-169.99) -173.879
(172.85) 174.840	(85.00) 82.583	(-167.97) -166.757
(-172.38) -172.351	(89.72) 83.582	(-164.52) -160.132
(-172.37) -172.912	(89.66) 83.020	(-164.00) -158.339
(172.44) 175.464	(86.51) 81.692	(-177.02) -173.212

Compound 25



Molecule (-707.8361617au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)

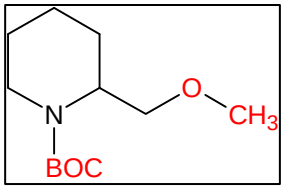
Conformer.1	-25.02602	0
Conformer.2	-22.397537	2.628483
Conformer.3	-21.025042	4.000978
Conformer.4	-19.104916	5.92110399

conformer energies nbp-2-m#		relative energies
Conformer.1	-707.8472858	0
Conformer.2	-707.8443433	0.0029425
Conformer.3	-707.8443437	0.0029421
Conformer.4	-707.8403939	0.0068919

Dih(O3,C6,C5,C4)	Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)
(172.45) -172.3476	(-76.71) -75.99736	(-53.00) -55.24799	(54.82) 55.13328
(-177.30) -146.5372	(173.26) -175.6852	(51.60) 57.95515	(-50.58) -58.12873
(-177.19) 178.9220	(173.26) 174.6216	(51.65) 51.5278	(-50.61) -51.50255
(176.51) -174.464	(-74.43) -73.55817	(-51.64) -54.26465	(52.82) 53.45101

Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C7)	Dih(C1,N1,C7,O2)	Dih(N1,C7,O2,C8)
(-54.30) -51.10353	(-145.91) -154.933	(14.97) 14.9035	(179.61) -178.654
(55.68) 52.29276	(106.23) 164.6968	(2.35) -20.45160	(177.43) -179.617
(55.72) 55.37176	(106.43) 98.55189	(2.37) 7.01668	(177.56) 179.650
(-53.88) -50.98703	(-132.45) -146.294	(0.65) 3.55751	(179.42) -179.486

Dih(C7,O2,C8,C10)	Dih(O1,C7,N1,C5)	Dih(O2,C7,N1,C5)	Dih(N1,C5,C6,O3)
(61.65) 62.678	(-5.93) -7.483	(175.34) 171.7737	(47.40) 62.0153
(-179.01) 179.9393	(-10.83) 10.3227	(169.74) -169.897	(56.83) 89.2692
(-178.98) 179.8467	(-10.54) -15.012	(170.01) 165.8305	(56.95) 53.3278
(179.63) 179.3612	(-9.95) -15.30260	(171.64) 165.9517	(52.74) 61.5052



Compound 27

Molecule (-746.8620650 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)
Conformer.1	-14.610275	0
Conformer.2	-13.624543	0.985731999
Conformer.3	-12.684909	1.925366
Conformer.4	-11.605637	3.004638
Conformer.5	-11.343882	3.266393
Conformer.6	-9.66939299	4.94088

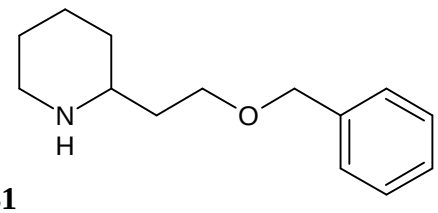
Conformation Energies		Relative Energies
Conformer.1	-746.8671541	0
Conformer.2	-746.8647077	0.0024464
Conformer.3	-746.8621037	0.0050504
Conformer.4	-746.8592061	0.007948
Conformer.5	-746.8591097	0.0080444
Conformer.6	-746.8671541	0

Dih(C7,O3,C6,C5)	Dih(O3,C6,C5,C4)	Dih(C6,C5,C4,31)	Dih(C5,C4,C3,C2)
(177.85) 179.0866	(61.00) 57.62906	(66.36) 69.69049	(36.09) 34.78462
(88.57) 81.2665	(59.62) 57.69129	(66.27) 70.29061	(35.67) 34.31479
(177.93) 176.6831	(176.43) 163.5546	(66.52) 67.35313	(31.69) 33.47227
(109.91) 107.8476	(176.87) 164.2482	(67.26) 67.69735	(30.86) 32.69931
(-90.01) -84.5336	(175.94) 165.7844	(65.26) 66.87198	(31.54) 32.92717
(177.95) -74.4753	(60.98) 105.99854	(66.36) 69.70704	(36.11) 30.59168

Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C8)	Dih(C1,N1,C8,O2)
(20.75) 19.64836	(-57.98) -56.14250	(-155.34) -151.186	(-176.75) -178.039
(21.10) 19.86308	(-58.14) -56.20469	(-154.86) -150.555	(-176.69) -178.290
(24.95) 21.01577	(-56.51) -54.39219	(-162.97) -155.620	(-169.28) -173.173
(25.84) 22.05464	(-56.99) -54.69091	(-166.96) -161.132	(-170.21) -173.878
(24.92) 21.35512	(-55.63) -53.72219	(-166.17) -158.435	(-170.55) -172.447
(20.73) 24.60268	(-57.98) -57.95957	(-155.31) -149.261	(-176.74) 179.461

Dih(N1,C8,O2,C9)	Dih(C8,O2,C9,C11)	Dih(O1,C8,N1,C5)	Dih(C8,N1,C5,C6)
(179.33) -179.877	(-179.38) -179.968	(171.14) 175.353	(86.91) 80.069
(179.54) -179.460	(62.91) 62.786	(171.58) 175.439	(86.86) 79.255
(-171.54) -176.898	(-66.73) -64.275	(177.20) 179.353	(95.10) 86.134
(-176.23) -179.858	(-64.22) -63.850	(173.20) 174.656	(99.00) 92.050
(178.48) 179.173	(-61.65) -62.373	(174.43) 178.052	(98.80) 89.105
(179.35) -178.266	(62.94) 62.359	(171.15) 177.233	(86.88) 79.107

Dih(N1,C5,C6,O3)
(-175.87) -177.293
(-177.53) -177.076
(-60.41) -73.000
(-59.42) -72.131
(-61.28) -70.955
(-175.89) -129.718



Compound 31

Molecule (-671.6838594 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	23.6795	0	0.03774	0
Conformer.2	23.9807	0.30116	0.03822	0.00048
Conformer.3	23.9826	0.30306	0.03822	0.00048
Conformer.4	25.7416	2.06206	0.04102	0.00329
Conformer.5	25.801	2.12151	0.04112	0.00338
Conformer.6	25.8155	2.13602	0.04114	0.0034
Conformer.7	25.9152	2.23567	0.0413	0.00356
Conformer.8	25.9528	2.27332	0.04136	0.00362
Conformer.9	26.0242	2.3447	0.04147	0.00374
Conformer.10	26.1986	2.51909	0.04175	0.00401
Conformer.11	26.2517	2.57222	0.04183	0.0041
Conformer.12	26.3008	2.62132	0.04191	0.00418
Conformer.13	27.8056	4.12612	0.04431	0.00658
Conformer.14	28.1071	4.42762	0.04479	0.00706
Conformer.15	28.1651	4.48563	0.04488	0.00715
Conformer.16	28.4118	4.73229	0.04528	0.00754
Conformer.17	28.4958	4.81634	0.04541	0.00768
Conformer.18	29.0893	5.40977	0.04636	0.00862
Conformer.19	30.3638	6.68434	0.04839	0.01065
Conformer.20	30.5312	6.85168	0.04865	0.01092
Conformer.21	30.6666	6.98708	0.04887	0.01113
Conformer.22	31.5038	7.82425	0.0502	0.01247
Conformer.23	32.0398	8.36032	0.05106	0.01332
Conformer.24	32.2199	8.54045	0.05135	0.01361
Conformer.25	32.6396	8.96012	0.05201	0.01428
Conformer.26	32.6875	9.00798	0.05209	0.01436
Conformer.27	32.8727	9.19323	0.05239	0.01465
Conformer.28	33.1512	9.47173	0.05283	0.01509
Conformer.29	33.2568	9.57733	0.053	0.01526
Conformer.30	33.5853	9.90576	0.05352	0.01579
Conformer.31	33.6195	9.94002	0.05358	0.01584

Conformation energies relative energies

-671.6842476	0
-671.6840332	0.000214
-671.6838594	0.000388
-671.6807817	0.003466
-671.6831423	0.001105

Dih(C9,C14,C13,C12)	Dih(C14,C13,C12,C11)	Dih(C13,C12,C11,C10)
(0.44) -0.2976	(-0.10) -0.0866	(-0.22) 0.07599
(-0.19) -0.3215	(0.22) -0.0769	(0.08) 0.07843
(0.30) -0.4778	(-0.05) -0.1465	(-0.19) 0.12561
(0.28) -0.4725	(-0.01) -0.1308	(-0.23) 0.1076
(-0.45) 0.28732	(0.11) 0.09108	(0.22) -0.0744
-0.3266	-0.0783	0.07385
-0.4543	-0.1228	0.10361
-0.4257	-0.117	0.14115
-0.5458	-0.1849	0.21081
-0.4768	-0.1496	0.1273
-0.1017	-0.0396	-0.0378
-0.4951	-0.2037	0.18234
-0.6945	-0.0898	0.23793
-0.1491	0.03074	-0.0356
-0.2677	-0.0884	0.06844
-0.4686	-0.1432	0.1146
-0.4013	-0.1587	0.13122
0.76215	0.33472	-0.3496
0.40408	0.09285	-0.0848
0.67201	0.30102	-0.2905
-0.3454	-0.0951	0.11459
-0.3035	-0.1197	0.09611
-0.4953	-0.1127	0.17476
-0.4748	-0.144	0.12392
-0.4672	-0.1544	0.1295
-0.2339	-0.0461	0.04092
-0.3787	-0.0979	0.11969
0.023	0.00069	-0.0259
-0.4754	-0.1457	0.12315
-0.4457	-0.1315	0.1307

0.34868	0.13027	-0.114

Dih(C11,C10,C9,C8)	Dih(C10,C9,C8,O1)	Dih(C9,C8,O1,C7)
(-178.03) -179.12	(-41.13) -47.454	(-75.14) -79.931
(-177.61) -178.96	(-140.97) -135.06	(75.56) 81.5997
(-178.19) -178.05	(-21.48) -37.862	(176.96) 179.942
(-177.94) -177.97	(-24.28) -38.651	(173.12) 174.794
(178.05) 179.076	(41.76) 47.9934	(174.49) 78.693
-178.89	-45.86	-82.859
-178.13	-39.26	178.844
-178.85	-139.19	80.2666
-178.7	-145.46	102.089
-178.07	-37.315	-177.71
-179.66	-57.301	-80.416
-178.72	-37.702	-101.16
-178.84	-145.08	76.2351
-178.91	-56.89	173.282
-179.15	-49.032	-76.49
-178.02	-29.407	175.768
-178.75	-41.376	-81.788
179.102	33.5293	100.887
178.17	45.6631	-179.14
178.81	31.4557	105.105
-179.05	-134.72	78.6121
-179.28	-47.144	-77.495
-178.93	-139.79	77.1647
-178.06	-38.376	-179.77
-178.27	-37.021	-175.75
-179.32	-49.437	-79.525
-178.95	-136.16	80.0581
179.159	-73.344	-80.731
-178.03	-39.081	-177.13
-178.76	-140.81	103.267
179.118	44.7218	78.6414

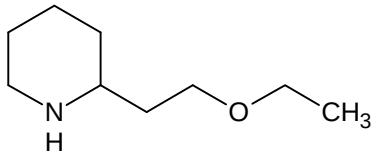
Dih(O1,C7,C6,C5)	Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)
(175.28) 178.878	(63.00) 63.8009	(-179.70) 179.595	(53.88) 53.2037

(179.50) -179.01	(65.44) 65.6675	(-179.77) 179.494	(53.82) 53.1109
(175.93) 179.516	(63.30) 64.6135	(-179.65) 179.664	(53.87) 53.1736
(175.56) 178.526	(60.83) 61.69	(-179.46) 179.941	(53.98) 53.3321
(-80.92) -82.376	(60.50) 58.1178	(-179.28) 178.974	(54.22) 53.6537
178.706	61.4393	179.847	53.3294
-82.541	57.5638	179.138	53.7011
177.754	64.9212	179.528	53.1394
-176.21	63.617	179.649	53.3058
177.877	65.652	179.57	53.0988
-85.311	57.4598	179.603	53.5646
173.968	64.1664	179.469	53.0974
77.1001	64.8189	177.439	52.7917
82.7964	74.2713	177.945	52.3956
86.3623	74.228	178.163	52.4213
-80.529	57.7169	179.099	53.632
-81.319	57.5244	179.028	53.6249
99.2762	-166.62	-177.83	53.0802
54.33	47.5267	178.618	53.2446
99.2238	-173.67	-74.322	-51.987
51.0951	46.6959	178.828	53.2157
-172.19	74.3156	-91.924	-47.868
179.6	51.0997	-89.152	-48.15
-173.26	73.5518	-92.065	-48.02
-74.654	50.6528	-89.782	-48.21
178.725	49.8747	-88.673	-48.214
-75.594	49.5483	-89.17	-48.26
-69.992	75.0292	-96.326	-45.125
-170.91	69.2252	-92.877	-47.376
-169.13	72.4434	-92.719	-47.39
-172.88	74.3163	-91.865	-47.602

Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)
(-53.17) -52.513	(55.73) 55.204	(-61.16) -58.381	(-173.61)-176.18
(-53.12) -52.366	(55.69) 55.108	(-61.18) -58.563	(-173.54)-176
(-53.16) -52.484	(55.72) 55.208	(-61.15) -58.438	(-173.64)-76.23
(-53.26) -52.702	(55.73) 55.243	(-61.01) -58.063	(-173.98)-176.6
(-53.60) -52.681	(55.74) 55.116	(-60.63) -58.026	(-173.82)-175.4

-52.673	55.1753	-58.055	-176.52
-52.783	55.1694	-57.888	-175.69
-52.476	55.1008	-58.337	-176.24
-52.685	55.2534	-58.103	-176.29
-52.423	55.1177	-58.451	-176.22
-52.937	55.2739	-57.658	-176.29
-52.375	55.1121	-58.533	-176.07
-51.834	54.718	-59.367	-173.77
-51.304	54.6165	-60.067	-173.73
-51.446	54.7387	-59.899	-174.11
-52.818	55.0892	-57.667	-175.85
-52.765	55.0504	-57.752	-175.72
-52.36	55.4261	-58.839	179.799
-52.934	55.2095	-57.683	-175.9
52.0953	-54.702	56.5142	71.7804
-53.101	55.3717	-57.372	-176.28
54.3964	-57.532	52.5133	90.3028
53.5435	-56.772	53.7493	87.3778
54.6468	-57.527	52.2296	90.6743
53.7083	-57.097	53.7085	89.0754
53.4421	-56.529	53.4233	87.4343
53.43	-56.869	53.9773	88.3201
53.5693	-58.888	53.9592	93.2784
54.6679	-57.932	52.3161	91.4554
54.4889	-57.862	52.4939	91.11
54.0785	-57.425	52.795	89.8589

Compound 30



Molecule (-481.1719656 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	Rel. E gas(au)	E gas(au)

Conformer.1	0.04862	0	0	7.75E-05
Conformer.2	0.74137	0.69274	0.0011	0.00118
Conformer.3	1.43264	1.38401	0.00221	0.00228
Conformer.4	1.5348	1.48617	0.00237	0.00245
Conformer.5	1.63064	1.58201	0.00252	0.0026
Conformer.6	1.74856	1.69993	0.00271	0.00279
Conformer.7	2.16463	2.11601	0.00337	0.00345
Conformer.8	2.23769	2.18906	0.00349	0.00357
Conformer.9	2.24899	2.20037	0.00351	0.00358
Conformer.10	2.4919	2.44327	0.00389	0.00397
Conformer.11	3.13913	3.09051	0.00493	0.005
Conformer.12	3.18116	3.13254	0.00499	0.00507
Conformer.13	3.29303	3.2444	0.00517	0.00525
Conformer.14	3.60106	3.55244	0.00566	0.00574
Conformer.15	3.60799	3.55936	0.00567	0.00575
Conformer.16	3.79984	3.75122	0.00598	0.00606
Conformer.17	3.88177	3.83315	0.00611	0.00619
Conformer.18	3.89011	3.84148	0.00612	0.0062
Conformer.19	3.94621	3.89759	0.00621	0.00629
Conformer.20	4.21651	4.16788	0.00664	0.00672
Conformer.21	4.61026	4.56164	0.00727	0.00735
Conformer.22	4.80973	4.7611	0.00759	0.00766
Conformer.23	5.03168	4.98305	0.00794	0.00802
Conformer.24	5.22111	5.17248	0.00824	0.00832
Conformer.25	5.33044	5.28181	0.00842	0.00849
Conformer.26	5.36981	5.32118	0.00848	0.00856
Conformer.27	5.39547	5.34684	0.00852	0.0086
Conformer.28	5.52746	5.47884	0.00873	0.00881
Conformer.29	5.53656	5.48794	0.00875	0.00882
Conformer.30	5.69213	5.6435	0.00899	0.00907
Conformer.31	5.72574	5.67712	0.00905	0.00912
Conformer.32	5.78611	5.73749	0.00914	0.00922
Conformer.33	5.87712	5.82849	0.00929	0.00937
Conformer.34	6.29765	6.24902	0.00996	0.01004
Conformer.35	6.48352	6.43489	0.01025	0.01033
Conformer.36	6.73361	6.68498	0.01065	0.01073
Conformer.37	7.1993	7.15068	0.0114	0.01147

Conformer.38	7.35399	7.30537	0.01164	0.01172
Conformer.39	7.52432	7.4757	0.01191	0.01199
Conformer.40	7.91435	7.86572	0.01253	0.01261
Conformer.41	9.01826	8.96963	0.01429	0.01437

Conformation energies	Relative energies
-481.1757887	0
-481.1749178	0.000871
-481.1731854	0.002603
-481.1730737	0.002715
-481.1731534	0.002635

Dih(C9,C8,O1,C7)	Dih(C8,O1,C7,C4)	Dih(O1,C7,C4,C3)	Dih(C7,C4,C3,C5)
(179.85) 179.834	(179.11)-179.98	(59.06) 55.8194	(62.81) 59.6898
(179.89) 179.848	(178.76) 179.588	(172.55) 173.182	(64.10) 61.8169
(79.97) 82.3341	(175.73) -179.26	(59.80) 56.1369	(63.14) 59.4692
(174.33) 178.011	(76.63) 78.3192	(52.65) 50.8861	(60.20) 60.5274
(-79.16) -79.096	(-176.13) -177.04	(58.86) 55.9614	(62.54) 59.7413
175.891	76.9603	167.673	61.4438
-179.52	-179.79	-77.679	65.3822
78.9971	176.573	173.211	61.7649
-80.271	-178.11	173.109	61.8577
-179.43	-84.772	177.675	62.9609
-177.93	-77.467	-69.458	67.5407
84.7082	83.1874	51.7686	60.5212
84.9881	83.607	169.517	61.8098
-81.576	-179.11	-78.366	65.2709
179.475	176.859	-68.473	170.487
79.3489	177.316	-78.019	65.3947
-179.89	-178.94	176.242	64.5713
-85.619	-87.363	176.177	62.5429
179.685	179.09	53.1508	57.3561
-179.55	-179.78	-78.66	65.0343
177.315	75.8875	48.9035	59.6107
-86.242	-82.426	-72.71	66.5252
-177.58	-81.699	-178.91	66.0623

175.502	76.6926	168.777	62.4069
81.4407	179.11	53.4614	57.067
-79.165	-176.06	176.183	64.5702
80.2634	178.81	176.252	64.4827
-79.959	-178.48	53.2944	57.431
178.19	-82.903	-73.446	66.6389
-81.731	-179.16	-79.278	65.1346
85.5343	88.9102	-176.12	176.99
73.2889	-111.47	-74.299	66.56
79.5918	177.568	-78.772	65.4213
83.6118	79.4897	48.5218	59.3884
-85.659	-86.254	178.684	65.1969
85.1306	84.1244	171.666	63.2903
-86.38	-84.387	-75.289	66.0032
172.304	78.8112	-106	174.358
69.3653	71.2894	-105.41	169.337
74.2868	-114.34	-76.492	65.619
85.3045	-169.62	97.0037	179.305

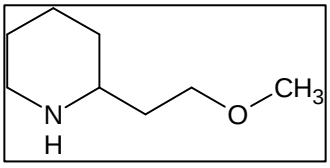
Dih(C4,C3,C5,C1)	Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)	Dih(C1,C6,C2,N1)
(175.04) 175.374	(-53.08) -52.268	(52.83) 52.1903	(-56.08) -55.971
(175.39) 175.889	(-52.87) -52.271	(52.69) 52.1003	(-55.98)-55.638
(175.06) 175.39	(-53.07) -52.262	(52.80) 52.1942	(-56.09) -55.972
(175.07) 175.337	(-52.89) -52.362	(52.82) 52.2896	(-56.10) -55.938
(175.03) 175.36	(-53.05) -52.267	(52.81) 52.1874	(-56.10) -55.969
175.678	-52.305	52.1618	-55.71
174.891	-52.017	52.4473	-56.157
175.888	-52.267	52.1001	-55.643
175.87	-52.265	52.103	-55.646
175.66	-52.312	52.2195	-55.708
174.342	-52.035	52.4106	-56.269
175.29	-52.345	52.2837	-55.96
175.65	-52.286	52.1457	-55.714
174.962	-52.036	52.4395	-56.135
74.0476	52.3916	-52.426	54.6586
174.928	-52.031	52.4393	-56.14
71.5504	52.6992	-51.703	54.0806

175.722	-52.311	52.213	-55.692
71.6283	53.5702	-52.442	53.8276
70.5288	53.3899	-51.638	53.7183
71.7374	53.1898	-52.32	54.0297
174.457	-52.022	52.4327	-56.255
71.4635	52.615	-51.699	54.1714
71.7529	52.9509	-52.002	53.97
71.6083	53.6032	-52.447	53.8051
71.5095	52.7194	-51.697	54.0646
71.5467	52.7127	-51.709	54.0735
71.6141	53.5675	-52.432	53.8246
70.4958	53.4677	-51.761	53.7118
70.6099	53.3439	-51.647	53.7593
74.3579	51.4817	-51.654	54.903
174.539	-52.013	52.448	-56.25
70.5669	53.3384	-51.628	53.7566
71.7221	53.2276	-52.33	54.0138
71.5376	52.6378	-51.726	54.1525
71.5723	52.9679	-51.933	53.9397
70.4909	53.5052	-51.779	53.673
74.3113	51.9285	-52.022	54.6858
177.694	-53.002	52.294	-55.42
70.3666	53.4977	-51.694	53.6544
74.9238	50.8977	-50.95	55.0921

Dih(C6,C2,N1,C3)		Dih(C2,N1,C3,C4)		Dih(N1,C3,C4,C7)	
(62.12)	59.7141	(176.06)	178.314	(-177.15)	-178.71
(62.07)	59.5787	(175.86)	177.924	(-175.52)	-176.32
(62.13)	59.7037	(176.07)	178.294	(-176.83)	-178.9
(62.04)	59.4861	(176.07)	178.628	(-179.49)	-177.83
(62.14)	59.7206	(176.05)	178.319	(-177.41)	-178.67
	59.5285		178.216		-176.79
	59.4113		178.288		-172.41
	59.582		177.917		-176.36
	59.5827		177.926		-176.28
	59.4413		178.246		-175.17
	59.6901		178.452		-170.73

59.5258	178.609	-177.85
59.5728	178.177	-176.45
59.3986	178.256	-172.5
-56.138	-72.019	-63.66
59.4115	178.264	-172.4
-56.955	-71.603	-169.88
59.4242	178.226	-175.56
-55.64	-73.075	-176.89
-56.671	-72.218	-169.25
-55.881	-72.886	-174.63
59.5909	178.481	-171.61
-56.999	-71.67	-168.43
-56.372	-72.29	-171.91
-55.614	-73.1	-177.15
-56.951	-71.592	-169.89
-56.942	-71.617	-169.97
-55.653	-73.051	-176.83
-56.503	-72.443	-167.85
-56.697	-72.228	-169.13
-57.454	-70.942	-56.771
59.5416	178.475	-171.49
-56.727	-72.18	-168.88
-55.865	-72.9	-174.85
-56.931	-71.739	-169.22
-56.474	-72.074	-171.13
-56.432	-72.423	-168.44
-56.681	-71.583	-59.574
59.0225	-179.66	-69.159
-56.528	-72.27	-168.81
-58.911	-69.563	-54.3

Compound 29



Molecule (-442.1318919 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	2.397837	0	0.00382	0
Conformer.2	3.015123	0.61729	0.0048	0.00098
Conformer.3	3.89672	1.49888	0.00621	0.00239
Conformer.4	4.002027	1.60419	0.00638	0.00256
Conformer.5	4.55941499	2.16158	0.00727	0.00344
Conformer.6	4.75470899	2.35687	0.00758	0.00376
Conformer.7	5.56244099	3.1646	0.00886	0.00504
Conformer.8	6.16079099	3.76295	0.00982	0.006
Conformer.9	6.29035599	3.89252	0.01002	0.0062
Conformer.10	6.64321199	4.24537	0.01059	0.00677
Conformer.11	6.96329299	4.56546	0.0111	0.00728
Conformer.12	7.29052099	4.89268	0.01162	0.0078
Conformer.13	7.48105899	5.08322	0.01192	0.0081
Conformer.14	8.06205599	5.66422	0.01285	0.00903
Conformer.15	9.62137899	7.22354	0.01533	0.01151

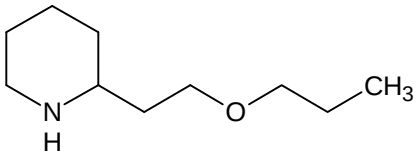
Conformation Energies	Relative Energies
-442.1357647	0
-442.1348965	0.000868
-442.1330272	0.002737
-442.1324223	0.003342
-442.1340839	0.001681

Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)	Dih(C1,C6,C2,N1)	Dih(C6,C2,N1,C3)
-52.26933	52.18776	-55.97080	59.72331
-52.27193	52.10044	-55.63815	59.57855
-52.35615	52.29168	-55.94419	59.49226
-52.30605	52.16344	-55.71077	59.52643
-52.04133	52.43982	-56.13501	59.40524
-52.31315	52.22221	-55.71192	59.44366

-52.06845	52.40864	-56.23319	59.64774
52.69632	-51.70464	54.08435	-56.95667
53.55778	-52.43194	53.83253	-55.65875
53.30550	-51.63514	53.78466	-56.73851
53.18677	-52.30958	54.02746	-55.89510
52.61064	-51.70129	54.17846	-57.00319
52.94807	-52.00729	53.97628	-56.37010
53.32150	-51.78199	53.82978	-56.57802
51.91247	-52.01049	54.69408	-56.70463

Dih(C2,N1,C3,C4)	Dih(N1,C3,C4,C7)
178.33034	-178.57485
177.92320	-176.31346
178.65214	-177.74448
178.21861	-176.78606
178.27478	-172.35311
178.25613	-175.06172
178.40436	-171.05620
-71.61029	-169.87226
-73.05239	-176.73911
-72.19327	-168.78788
-72.86997	-174.50452
-71.67627	-168.31707
-72.31092	-171.92667
-72.49633	-167.54629
-71.55990	-59.42294

Compound 32



Molecule (-520.2068929 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	-0.2887	0	-0.00046	0
Conformer.2	-0.2563	0.032358	-0.000408	5.16E-05
Conformer.3	-0.108	0.180651	-0.000172	0.00029
Conformer.4	-0.0366	0.252131	-5.83E-05	0.0004
Conformer.5	0.16849	0.457178	0.0002685	0.00073
Conformer.6	0.16936	0.45805	0.0002699	0.00073
Conformer.7	0.41846	0.707151	0.0006669	0.00113
Conformer.8	0.62344	0.912129	0.0009935	0.00145
Conformer.9	0.62375	0.91244	0.000994	0.00145
Conformer.10	0.92182	1.210508	0.001469	0.00193
Conformer.11	1.12964	1.418331	0.0018002	0.00226
Conformer.12	1.18018	1.468867	0.0018807	0.00234
Conformer.13	1.33778	1.62647	0.0021319	0.00259
Conformer.14	1.36296	1.651651	0.002172	0.00263
Conformer.15	1.41726	1.705951	0.0022586	0.00272
Conformer.16	1.419	1.707683	0.0022613	0.00272
Conformer.17	1.47355	1.76224	0.0023483	0.00281
Conformer.18	1.5209	1.809589	0.0024237	0.00288
Conformer.19	1.55362	1.842303	0.0024758	0.00294
Conformer.20	1.56497	1.853658	0.0024939	0.00295
Conformer.21	1.59305	1.881733	0.0025387	0.003
Conformer.22	1.60799	1.896678	0.0025625	0.00302
Conformer.23	1.65942	1.948105	0.0026444	0.0031
Conformer.24	1.6658	1.954488	0.0026546	0.00311

Conformer.25	1.82194	2.110624	0.0029034	0.00336
Conformer.26	1.84168	2.130366	0.0029349	0.00339
Conformer.27	1.84337	2.132054	0.0029376	0.0034
Conformer.28	1.95528	2.243971	0.0031159	0.00358
Conformer.29	1.97913	2.267815	0.0031539	0.00361
Conformer.30	1.98467	2.273357	0.0031628	0.00362
Conformer.31	1.98637	2.275059	0.0031655	0.00363
Conformer.32	2.16336	2.45205	0.0034475	0.00391
Conformer.33	2.4129	2.701582	0.0038452	0.00431
Conformer.34	2.42381	2.712496	0.0038626	0.00432
Conformer.35	2.51713	2.805815	0.0040113	0.00447
Conformer.36	2.52656	2.815247	0.0040263	0.00449
Conformer.37	2.71112	2.999807	0.0043204	0.00478
Conformer.38	2.88253	3.171215	0.0045936	0.00505
Conformer.39	2.90308	3.191765	0.0046263	0.00509
Conformer.40	2.92649	3.215173	0.0046636	0.00512
Conformer.41	2.95721	3.245892	0.0047126	0.00517
Conformer.42	2.97715	3.265832	0.0047444	0.0052
Conformer.43	2.99033	3.27902	0.0047654	0.00523
Conformer.44	3.02641	3.315099	0.0048229	0.00528
Conformer.45	3.0319	3.320589	0.0048316	0.00529
Conformer.46	3.07931	3.367994	0.0049072	0.00537
Conformer.47	3.1801	3.468785	0.0050678	0.00553
Conformer.48	3.27423	3.562919	0.0052178	0.00568
Conformer.49	3.41457	3.703253	0.0054415	0.0059
Conformer.50	3.50648	3.79517	0.0055879	0.00605
Conformer.51	3.52873	3.817412	0.0056234	0.00608
Conformer.52	3.55848	3.84717	0.0056708	0.00613
Conformer.53	3.72307	4.011757	0.0059331	0.00639
Conformer.54	3.75461	4.043296	0.0059833	0.00644
Conformer.55	3.76166	4.050351	0.0059946	0.00645
Conformer.56	3.79126	4.079945	0.0060417	0.0065
Conformer.57	3.84474	4.133427	0.006127	0.00659
Conformer.58	3.86917	4.157858	0.0061659	0.00663
Conformer.59	3.91065	4.199341	0.006232	0.00669
Conformer.60	3.98582	4.274507	0.0063518	0.00681
Conformer.61	3.99826	4.286946	0.0063716	0.00683

Conformer.62	4.00597	4.294654	0.0063839	0.00684
Conformer.63	4.01845	4.307136	0.0064038	0.00686
Conformer.64	4.05607	4.344753	0.0064637	0.00692
Conformer.65	4.16314	4.451832	0.0066344	0.00709
Conformer.66	4.19704	4.485728	0.0066884	0.00715
Conformer.67	4.25832	4.547007	0.0067861	0.00725
Conformer.68	4.49725	4.785935	0.0071668	0.00763
Conformer.69	4.50183	4.790521	0.0071741	0.00763
Conformer.70	4.5201	4.808792	0.0072032	0.00766
Conformer.71	4.55263	4.841316	0.0072551	0.00772
Conformer.72	4.56763	4.856319	0.007279	0.00774
Conformer.73	4.75725	5.045933	0.0075811	0.00804
Conformer.74	4.86476	5.153449	0.0077525	0.00821
Conformer.75	4.88428	5.172968	0.0077836	0.00824
Conformer.76	4.94145	5.230141	0.0078747	0.00833
Conformer.77	4.94735	5.236039	0.0078841	0.00834
Conformer.78	4.95606	5.244746	0.007898	0.00836
Conformer.79	5.06642	5.355103	0.0080738	0.00853
Conformer.80	5.07751	5.366199	0.0080915	0.00855
Conformer.81	5.13506	5.423746	0.0081832	0.00864
Conformer.82	5.13727	5.425958	0.0081868	0.00865
Conformer.83	5.13742	5.426105	0.008187	0.00865
Conformer.84	5.17521	5.463897	0.0082472	0.00871
Conformer.85	5.21897	5.50766	0.008317	0.00878
Conformer.86	5.36443	5.653116	0.0085488	0.00901
Conformer.87	5.50901	5.797698	0.0087792	0.00924
Conformer.88	5.58044	5.869127	0.008893	0.00935
Conformer.89	5.58228	5.870968	0.0088959	0.00936
Conformer.90	6.27883	6.567519	0.0100059	0.01047
Conformer.91	6.43282	6.721506	0.0102513	0.01071
Conformer.92	6.51891	6.807601	0.0103885	0.01085
Conformer.93	6.7582	7.046883	0.0107699	0.01123
Conformer.94	6.92218	7.210864	0.0110312	0.01149
Conformer.95	6.9815	7.270188	0.0111257	0.01159
Conformer.96	7.27066	7.559347	0.0115865	0.01205
Conformer.97	7.64882	7.937506	0.0121892	0.01265
Conformer.98	7.70756	7.996243	0.0122828	0.01274

Conformer.99	7.9584	8.247084	0.0126825	0.01314
Conformer.100	9.00455	9.293236	0.0143497	0.01481

Conformation Energies	Relative energies
-520.2104972	0.0002847
-520.2106334	0.0001485
-520.2107000	0.0000819
-520.2105460	0.0002359
-520.2107819	0

Dih(C10,C9,C8,O1)	Dih(C9,C8,O1,C7)	Dih(C8,O1,C7,C6)	Dih(O1,C7,C6,C5)
(179.94) -179.94	(179.92) 179.804	(179.15) -179.89	(59.26) 55.7631
(-63.20) -63.295	(178.90) 178.384	(178.23) -179.12	(58.83) 54.8365
(62.75) 63.4814	(-179.00) 179.793	(179.25) 179.806	(59.27) 55.6202
(-179.96) -180	(-179.75) -179.81	(-178.97) -179.35	(-175.71) -175.32
(-62.67) -63.656	(179.41) 179.944	(-179.23) -179.33	(-175.51) -175.36
63.659	-179.57	-179.38	-175.29
-180	179.846	179.585	173.182
63.6559	-179.9	179.567	173.223
-63.653	179.608	179.619	173.157
58.79	84.0307	-177.13	57.7205
63.662	-179.44	79.0298	49.8453
-179.99	178.169	78.253	50.7031
-174.66	-80.909	-177.6	55.9061
-56.088	-77.712	-177.19	55.8887
-63.555	178.029	78.3411	50.7589
-179.93	175.939	77.0217	167.647
179.953	179.489	176.666	-69.221
175.1	82.8334	179.532	-175.21
55.9383	78.7204	178.473	-175.34
63.4157	-179.53	176.169	-68.665
179.846	-179.48	-84.338	-172.94
63.9322	177.851	78.6186	167.773

-63.758	175.274	76.4403	167.601
-63.57	179.424	176.883	-69.144
179.911	-179.47	-179.89	-77.646
62.9249	179.091	179.482	-79.05
63.5762	-178.98	-83.942	-172.79
-174.98	-82.243	-178.9	173.087
56.0116	77.2798	176.503	173.133
-55.937	-78.176	-177.86	173.261
-63.357	-179.24	-179.43	-77.275
179.795	-179.68	-85.016	177.602
63.5132	-179.13	-84.635	177.789
-63.476	-179.43	87.38	-177.68
-63.619	-177.97	179.7	67.6997
62.7181	178.834	178.924	65.3223
-56.58	-81.34	175.294	-68.244
-176.17	-85.832	172.905	-69.128
175.048	82.278	179.793	176.668
175.289	83.5535	-179.57	54.3479
-179.95	179.939	-179.49	56.2717
-180	179.962	179.494	-175.7
57.8319	83.1474	83.1717	51.5961
-63.356	178.833	-178.95	55.5267
-176.95	-86.431	-87.677	-174.58
56.2472	75.25	172.015	-69.153
63.6388	-179.81	179.443	-175.68
-175.61	-83.481	-179.98	-78.419
-55.991	-72.695	-170.37	-73.916
174.654	81.2278	177.914	-77.959
56.1043	78.0614	177.529	-77.881
179.998	-179.89	-178.95	176.246
58.5011	84.0685	89.3916	-176.65
63.6463	-179.59	-178.99	176.326
-63.635	179.882	-178.9	176.233
63.4787	179.666	178.874	52.958
62.6131	178.598	179.22	-80.576
179.908	-179.51	-179.87	-78.651
63.3774	-179.03	179.35	-58.944

-63.03	-178.97	-179.03	-78.154
63.9548	173.424	84.495	68.0973
-63.521	-179.98	-179.97	-59.418
179.866	179.832	-84.082	-65.12
-63.014	-176.15	86.4841	65.0305
-56.141	-79.416	-178.94	65.6413
58.2523	82.8683	-177.76	57.8879
63.4356	-179.94	-84.029	-65.046
174.824	81.6083	177.755	-175.6
55.7548	77.6064	176.989	-175.86
-174.91	-81.776	-178.75	-175.76
-56.035	-78.013	-177.92	-175.68
-63.581	177.573	77.0162	49.7854
63.6491	-177.2	-80.571	-170.83
-64.062	179.741	-83.692	-179.45
-179.95	175.554	76.7636	168.799
-179.93	-179.24	-173.61	90.7868
63.6135	-176.97	-81.199	-178.68
-63.279	179.466	-172.65	89.6321
-57.23	-81.346	178.488	-60.053
-174.69	-81.101	-176.8	176.17
63.567	-179.24	-173.9	90.6182
-179.97	177.744	-82.71	-72.973
56.0565	78.3264	178.638	176.187
-63.756	-179.7	-77.639	-49.506
-175.61	-84.183	177.665	-59.489
-175.6	-83.612	-180	-79.335
-177.02	-86.574	-87.489	-67.296
174.691	81.5186	178.217	-78.723
56.0794	78.6047	178.177	-78.543
176.511	86.0824	-170.14	91.0874
63.2467	87.0479	-174.56	94.9529
-56.762	-73.442	-167.16	90.8843
103.445	-68.09	-68.891	-178.98
-105.15	68.8222	71.3776	178.96
-57.523	-82.417	-81.254	-50.884
-103.43	75.8009	172.255	56.023

63.8278	176.162	71.8047	64.1118
179.981	176.656	71.6743	63.7187
-63.557	176.06	71.711	64.9474
-105.76	72.0876	69.3185	50.1004

Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)
(63.21) 59.654	(175.11) 175.379	(-53.09) -52.268	(52.81) 52.1909
(62.03) 59.1676	(175.05) 175.472	(-53.04) -52.279	(52.81) 52.1988
(63.18) 59.654	(175.11) 175.389	(-53.08) -52.27	(52.79) 52.1899
(174.50) 175.748	(177.94) 177.999	(-52.93) -52.366	(52.40) 51.8604
(174.45) 175.746	(178.00) 177.997	(-52.92) -52.366	(52.38) 51.8606
175.748	177.999	-52.366	51.8603
61.814	175.888	-52.271	52.1003
61.8212	175.886	-52.271	52.1002
61.8144	175.889	-52.271	52.1
61.1625	175.754	-52.477	52.1089
60.2065	175.489	-52.384	52.2824
60.5187	175.35	-52.364	52.2885
59.7345	175.36	-52.267	52.1881
59.7236	175.365	-52.267	52.1874
60.4809	175.347	-52.362	52.29
61.4433	175.677	-52.305	52.1616
169.759	178	-52.353	51.3758
175.712	177.999	-52.369	51.8624
175.727	177.991	-52.37	51.8666
169.796	178.04	-52.35	51.3641
173.998	178.07	-52.296	51.633
61.4679	175.68	-52.303	52.1581
61.4307	175.676	-52.305	52.163
169.74	178	-52.353	51.3759
65.355	174.886	-52.013	52.4486
64.0425	174.839	-51.921	52.4733
174.015	178.072	-52.295	51.6324
61.8529	175.868	-52.264	52.1026
61.7549	175.891	-52.267	52.0997

61.8766	175.859	-52.262	52.104
65.4813	174.838	-52.002	52.4511
62.9393	175.663	-52.311	52.219
62.9861	175.656	-52.311	52.2198
176.162	177.996	-52.384	51.9219
169.052	75.5356	52.6843	-53.019
168.859	75.4633	52.7194	-53.01
170.659	178.216	-52.316	51.2985
170.103	178.062	-52.338	51.3585
64.4175	175.496	-52.081	52.1025
58.056	175.877	-51.969	51.7583
59.4192	71.5503	53.6555	-52.296
171.796	74.392	52.378	-51.899
60.4791	175.298	-52.345	52.2843
58.9511	71.5646	53.6966	-52.326
173.857	178.051	-52.305	51.6443
169.907	177.989	-52.357	51.3913
171.791	74.3891	52.3785	-51.9
65.275	174.968	-52.037	52.438
70.2837	175.098	-52.35	52.3094
65.3953	174.923	-52.029	52.44
65.4217	174.907	-52.025	52.4411
64.5651	71.548	52.7007	-51.703
176.295	177.994	-52.38	51.9211
64.5754	71.5347	52.7033	-51.7
64.5707	71.547	52.699	-51.702
57.3128	71.6346	53.5708	-52.446
62.9863	70.5392	53.5711	-51.706
64.9442	70.5171	53.4032	-51.639
174.625	74.0144	52.0171	-51.467
64.7915	70.3799	53.4794	-51.622
168.087	75.9005	52.7648	-53.249
174.353	73.9923	52.0513	-51.487
168.711	178.011	-52.345	51.3164
169.368	75.7996	52.6613	-53.072
168.397	75.4451	52.7643	-53.05
60.4283	71.6115	53.5165	-52.245

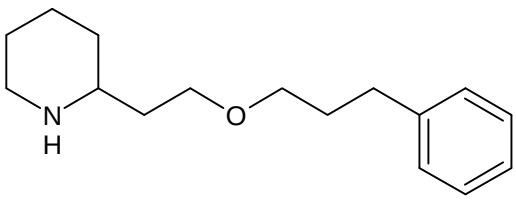
168.728	178.014	-52.344	51.3149
171.865	74.3762	52.368	-51.876
171.923	74.3477	52.3592	-51.857
171.838	74.3961	52.3709	-51.894
171.835	74.3927	52.3709	-51.894
59.2255	71.8863	53.5891	-52.46
172.446	74.3867	52.2855	-51.85
65.879	71.4637	52.6181	-51.698
62.4083	71.7412	52.954	-51.999
-177.8	177.412	-52.774	53.1063
66.1304	71.4532	52.615	-51.697
-177.39	177.358	-52.792	53.166
174.409	73.9958	52.0511	-51.478
64.5535	71.5017	52.7243	-51.697
-177.78	177.402	-52.777	53.1135
66.7266	70.4294	53.4922	-51.747
64.4687	71.5448	52.7135	-51.709
177.626	74.3131	51.672	-51.323
174.926	74.0417	51.988	-51.448
65.1082	70.6048	53.3477	-51.646
168.64	177.996	-52.346	51.3208
65.3902	70.557	53.3463	-51.629
65.3742	70.5008	53.3721	-51.621
-177.79	177.451	-52.76	53.0711
-178.59	177.418	-52.725	52.9612
-177.97	177.454	-52.765	53.076
64.1184	175.532	-52.319	52.2392
175.437	178.032	-52.39	51.9078
177.144	74.2373	51.7336	-51.322
59.0852	71.4904	53.7207	-52.311
163.416	178.582	-52.502	51.5559
163.254	178.63	-52.505	51.554
164.175	178.618	-52.509	51.6059
59.5258	71.8884	53.5603	-52.444

Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,C7)
(-56.08) -55.971	(62.11) 59.7121	(176.07)178.311	(-176.75) -178.74
(-56.10) -55.961	(62.09) 59.6798	(176.05) 178.242	(-177.86) -179.15
(-56.08) -55.969	(62.12) 59.7108	(176.05) 178.307	(-176.77) -178.73
(-53.23) -55.448	(54.30) 59.0706	(-179.42) 179.12	(-59.68) -61.79
(-53.25) -55.448	(54.35) 59.0704	(-179.50) 179.123	(-59.71) -61.793
-55.448	59.0703	179.121	-61.79
-55.639	59.5786	177.924	-176.32
-55.639	59.5791	177.926	-176.31
-55.638	59.5782	177.924	-176.32
-55.803	59.7573	178.113	-177.39
-55.916	59.4734	178.506	-178.08
-55.935	59.4839	178.621	-177.83
-55.97	59.7196	178.32	-178.67
-55.968	59.7183	178.318	-178.68
-55.937	59.4828	178.621	-177.86
-55.71	59.5287	178.218	-176.79
-55.404	59.9331	178.35	-68.607
-55.447	59.0701	179.128	-61.83
-55.447	59.065	179.14	-61.816
-55.398	59.9439	178.3	-68.556
-55.406	59.4208	178.608	-63.75
-55.708	59.5337	178.209	-176.77
-55.71	59.5262	178.221	-176.8
-55.404	59.9321	178.35	-68.625
-56.159	59.4109	178.289	-172.43
-56.205	59.3421	178.356	-173.6
-55.406	59.4214	178.605	-63.731
-55.647	59.5843	177.926	-176.28
-55.642	59.5809	177.915	-176.37
-55.649	59.5843	177.936	-176.26
-56.174	59.4248	178.309	-172.32
-55.707	59.4407	178.245	-175.19
-55.709	59.4425	178.248	-175.15
-55.414	58.9805	179.262	-61.328
55.0137	-56.06	-73.243	-64.197
54.9858	-56.057	-73.164	-64.442

-55.365	60.0106	178.071	-67.637
-55.394	59.9417	178.27	-68.224
-55.78	59.1806	178.649	-173.36
-55.851	59.7633	177.653	-179.88
53.5511	-56.029	-72.153	-175.3
54.3367	-57.209	-70.438	-62.436
-55.959	59.5221	178.606	-177.89
53.5323	-55.968	-72.229	-175.72
-55.407	59.4069	178.644	-63.898
-55.409	59.9109	178.391	-68.449
54.3361	-57.207	-70.437	-62.441
-56.133	59.3983	178.253	-172.5
-55.979	59.6451	178.164	-168.07
-56.143	59.4122	178.265	-172.4
-56.147	59.4159	178.273	-172.38
54.0794	-56.954	-71.602	-169.89
-55.416	58.9757	179.251	-61.185
54.075	-56.954	-71.591	-169.89
54.0795	-56.954	-71.599	-169.89
53.829	-55.634	-73.081	-176.92
53.5966	-56.427	-72.42	-171.14
53.7083	-56.659	-72.224	-169.34
54.1759	-57.784	-69.222	-60.298
53.6387	-56.615	-72.193	-169.52
55.0192	-55.757	-73.766	-65.109
54.1604	-57.741	-69.249	-60.581
-55.335	60.0317	178.245	-69.75
54.9511	-55.988	-73.341	-63.942
54.98	-55.985	-73.242	-64.897
53.6435	-56.199	-72.026	-174.36
-55.334	60.0332	178.24	-69.732
54.3302	-57.243	-70.379	-62.382
54.3237	-57.266	-70.328	-62.342
54.3385	-57.219	-70.428	-62.394
54.3372	-57.216	-70.426	-62.398
53.6877	-55.815	-72.641	-175.28
54.2169	-57.12	-70.406	-61.925

54.1627	-56.99	-71.662	-168.61
53.965	-56.371	-72.281	-171.92
-55.477	57.1027	-177.9	-54.411
54.1713	-57.003	-71.662	-168.37
-55.474	57.0067	-177.76	-53.971
54.1586	-57.758	-69.227	-60.523
54.0605	-56.948	-71.589	-169.91
-55.478	57.0929	-177.88	-54.398
53.6882	-56.501	-72.417	-167.8
54.072	-56.939	-71.616	-169.98
54.2838	-58.07	-69.175	-57.131
54.189	-57.82	-69.202	-59.983
53.7555	-56.694	-72.227	-169.16
-55.343	60.0293	178.26	-69.824
53.7511	-56.721	-72.182	-168.91
53.7267	-56.709	-72.159	-168.95
-55.463	57.1515	-178.01	-54.413
-55.432	57.3255	-178.24	-55.339
-55.485	57.1566	-177.97	-54.601
-55.753	59.4748	178.303	-174.08
-55.401	59.0166	179.242	-62.082
54.2427	-58.052	-69.113	-57.676
53.5114	-55.971	-72.203	-175.62
-55.195	59.8113	178.822	-74.832
-55.226	59.8251	178.821	-74.982
-55.233	59.7383	178.927	-73.994
53.7032	-55.84	-72.637	-174.98

Compound 33



Molecule (-749.7511473 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	18.6311	0	0.02969	0
Conformer.2	19.3671	0.73601	0.03086	0.00117
Conformer.3	19.6064	0.97535	0.03124	0.00155
Conformer.4	19.6724	1.04138	0.03135	0.00166
Conformer.5	19.9034	1.27232	0.03172	0.00203
Conformer.6	19.9607	1.32966	0.03181	0.00212
Conformer.7	20.0277	1.39668	0.03192	0.00223
Conformer.8	20.0909	1.45985	0.03202	0.00233
Conformer.9	20.3669	1.73586	0.03246	0.00277
Conformer.10	20.3753	1.74422	0.03247	0.00278
Conformer.11	20.7539	2.12287	0.03307	0.00338
Conformer.12	20.8154	2.18431	0.03317	0.00348
Conformer.13	20.8213	2.1902	0.03318	0.00349
Conformer.14	20.9416	2.31053	0.03337	0.00368
Conformer.15	21.0278	2.39671	0.03351	0.00382
Conformer.16	21.122	2.49092	0.03366	0.00397
Conformer.17	21.1281	2.49708	0.03367	0.00398
Conformer.18	21.1331	2.50206	0.03368	0.00399
Conformer.19	21.2694	2.63837	0.03389	0.0042
Conformer.20	21.3194	2.68839	0.03397	0.00428
Conformer.21	21.3439	2.71281	0.03401	0.00432
Conformer.22	21.6068	2.9758	0.03443	0.00474
Conformer.23	21.6192	2.98815	0.03445	0.00476
Conformer.24	21.6383	3.00723	0.03448	0.00479
Conformer.25	21.6767	3.04567	0.03454	0.00485
Conformer.26	21.7607	3.12968	0.03468	0.00499
Conformer.27	21.7708	3.13977	0.03469	0.005
Conformer.28	21.8624	3.23135	0.03484	0.00515
Conformer.29	21.87	3.23894	0.03485	0.00516
Conformer.30	21.8744	3.24334	0.03486	0.00517
Conformer.31	21.8847	3.25366	0.03488	0.00519
Conformer.32	21.9178	3.28671	0.03493	0.00524
Conformer.33	21.9343	3.30329	0.03495	0.00526
Conformer.34	21.9553	3.32428	0.03499	0.0053
Conformer.35	21.9746	3.34355	0.03502	0.00533
Conformer.36	22.0127	3.3816	0.03508	0.00539

Conformer.37	22.0731	3.44203	0.03518	0.00549
Conformer.38	22.0902	3.45919	0.0352	0.00551
Conformer.39	22.4196	3.78857	0.03573	0.00604
Conformer.40	22.487	3.85597	0.03584	0.00614
Conformer.41	22.498	3.86695	0.03585	0.00616
Conformer.42	22.5309	3.89983	0.03591	0.00621
Conformer.43	22.5327	3.90169	0.03591	0.00622
Conformer.44	22.6588	4.02779	0.03611	0.00642
Conformer.45	22.7911	4.16002	0.03632	0.00663
Conformer.46	22.8712	4.24017	0.03645	0.00676
Conformer.47	23.0461	4.41501	0.03673	0.00704
Conformer.48	23.0914	4.46034	0.0368	0.00711
Conformer.49	23.1231	4.49207	0.03685	0.00716
Conformer.50	23.1549	4.52388	0.0369	0.00721
Conformer.51	23.3683	4.73729	0.03724	0.00755
Conformer.52	23.4459	4.81488	0.03736	0.00767
Conformer.53	23.4465	4.81549	0.03736	0.00767
Conformer.54	23.5077	4.87661	0.03746	0.00777
Conformer.55	23.582	4.95091	0.03758	0.00789
Conformer.56	23.6127	4.98162	0.03763	0.00794
Conformer.57	23.6573	5.02628	0.0377	0.00801
Conformer.58	23.6875	5.05643	0.03775	0.00806
Conformer.59	23.7345	5.10341	0.03782	0.00813
Conformer.60	23.7688	5.13773	0.03788	0.00819
Conformer.61	23.8108	5.17978	0.03794	0.00825
Conformer.62	23.84	5.20891	0.03799	0.0083
Conformer.63	23.9399	5.30885	0.03815	0.00846
Conformer.64	23.9541	5.3231	0.03817	0.00848
Conformer.65	23.9839	5.35286	0.03822	0.00853
Conformer.66	24.0303	5.39926	0.03829	0.0086
Conformer.67	24.0425	5.41147	0.03831	0.00862
Conformer.68	24.0494	5.41833	0.03833	0.00863
Conformer.69	24.1264	5.49537	0.03845	0.00876
Conformer.70	24.2741	5.6431	0.03868	0.00899
Conformer.71	24.2976	5.66652	0.03872	0.00903
Conformer.72	24.3113	5.68024	0.03874	0.00905
Conformer.73	24.417	5.78595	0.03891	0.00922

Conformer.74	24.5117	5.88063	0.03906	0.00937
Conformer.75	24.5181	5.88707	0.03907	0.00938
Conformer.76	24.5263	5.89522	0.03909	0.00939
Conformer.77	24.5702	5.93916	0.03916	0.00946
Conformer.78	24.6724	6.0413	0.03932	0.00963
Conformer.79	24.7114	6.08036	0.03938	0.00969
Conformer.80	24.7933	6.16226	0.03951	0.00982
Conformer.81	24.891	6.25996	0.03967	0.00998
Conformer.82	24.9442	6.31318	0.03975	0.01006
Conformer.83	25.0747	6.44364	0.03996	0.01027
Conformer.84	25.093	6.46192	0.03999	0.0103
Conformer.85	25.1288	6.49776	0.04005	0.01035
Conformer.86	25.1746	6.54352	0.04012	0.01043
Conformer.87	25.2521	6.62106	0.04024	0.01055
Conformer.88	25.2533	6.62225	0.04024	0.01055
Conformer.89	25.3415	6.71047	0.04038	0.01069
Conformer.90	25.607	6.97594	0.04081	0.01112
Conformer.91	25.6486	7.01757	0.04087	0.01118
Conformer.92	25.7424	7.11135	0.04102	0.01133
Conformer.93	25.7924	7.16137	0.0411	0.01141
Conformer.94	25.8067	7.17566	0.04113	0.01144
Conformer.95	25.9558	7.32474	0.04136	0.01167
Conformer.96	26.0267	7.39567	0.04148	0.01179
Conformer.97	26.4019	7.77084	0.04207	0.01238
Conformer.98	26.9562	8.32511	0.04296	0.01327
Conformer.99	27.6411	9.01009	0.04405	0.01436
Conformer.100	28.4008	9.76974	0.04526	0.01557

Conformation Energy	Relative Energies
-749.756732	0.000106
-749.7567381	0.0001
-749.7553495	0.001489
-749.755331	0.001508
-749.7568385	0

Dih(C17,C16,C15,C14)	Dih(C16,C15,C14,C13)	Dih(C15,C14,C13,C12)
(-0.06) -0.0902	(-0.09) -0.0135	(0.09) 0.0702
(-0.06) 0.08859	(-0.05) 0.006326	(0.06) -0.0333
(-0.10) -0.1066	(-0.13) -0.07631	(0.11) 0.09058
(-0.12) -0.0762	(-0.12) -0.08646	(0.12) 0.07245
(-0.03) 0.21723	(-0.07) 0.080966	(0.04) -0.0885
0.08151	0.003626	-0.0263
0.04104	0.020398	-0.005
0.20389	0.084996	-0.0787
-0.0797	-0.09531	0.07284
0.23447	0.122239	-0.1212
-0.0899	-0.09678	0.08845
0.20638	0.080138	-0.0763
0.2171	0.080245	-0.0868
0.02739	0.019168	0.00337
-0.0595	-0.06462	0.07626
0.00093	-0.03939	0.03245
-0.1011	-0.07224	0.08467
0.2345	0.128612	-0.1261
0.20783	0.09014	-0.0855
0.05512	0.096097	-0.0456
0.04029	0.024191	-0.005
0.21475	0.077223	-0.081
-0.0182	-0.0772	0.05572
-0.0785	-0.09086	0.07379
-0.7199	0.081242	0.31214
-0.1222	-0.07209	0.0935
0.20382	0.08569	-0.0794
0.23753	0.120904	-0.1231
0.06279	-4.89E-05	-0.0135
0.22692	0.093825	-0.1022
0.21796	0.083527	-0.0892
0.20729	0.082234	-0.0795

-0.1064	-0.05679	0.09405
0.05676	0.091764	-0.0442
-0.1438	-0.03769	0.03988
0.19477	0.058831	-0.0515
0.20839	0.058291	-0.0622
0.21355	0.076068	-0.0786
0.20044	0.099319	-0.0863
-0.1057	-0.0571	0.07074
0.22739	0.090133	-0.1038
0.23919	0.127015	-0.1287
0.07057	0.005152	-0.0225
-0.1873	-0.08552	0.13293
0.20974	0.071474	-0.0788
0.24049	0.127586	-0.1304
0.0838	0.006694	-0.0289
0.03934	0.026412	-0.0058
-0.0253	-0.07386	0.05784
0.2068	0.063696	-0.0646
0.03822	0.041996	-0.0112
-0.076	-0.08816	0.07056
-0.1027	-0.07398	0.08717
-0.1268	-0.07112	0.09495
-0.0789	-0.09273	0.07137
0.20869	0.052744	-0.059
-0.2281	0.013955	0.0533
0.22858	0.085926	-0.1005
-0.0769	-0.08571	0.07425
-0.1347	0.057898	0.02998
0.21838	0.083287	-0.0906
-0.1081	-0.07145	0.08708
0.21376	0.075936	-0.0797
0.20968	0.076072	-0.0751
-0.0893	-0.13581	0.07756
0.03163	0.013261	0.00279
0.19934	0.103773	-0.0897
0.21616	0.077888	-0.0835
-0.0699	-0.05645	0.0622

0.24025	0.127492	-0.1301
-0.19	-0.11132	0.15533
0.23122	0.128031	-0.1232
0.00379	0.076995	-0.1149
-0.0944	-0.1011	0.09986
0.2379	0.122074	-0.1238
0.02812	0.008951	0.00544
-0.0014	0.042474	-0.075
-0.0962	-0.06793	0.08173
-0.0825	-0.10716	0.07449
-0.0893	-0.07555	0.07856
-0.1361	0.020112	0.00779
0.0836	0.005473	-0.0301
0.05396	0.107758	-0.0507
0.15223	0.043869	-0.0917
0.05884	0.085682	-0.0424
0.20971	0.048012	-0.0575
-0.0397	-0.07401	0.06513
-0.3842	-0.15251	0.03588
0.23658	0.12449	-0.1247
-0.4948	0.086903	0.12497
0.1962	0.10438	-0.0888
0.06503	0.392952	-0.4131
0.22849	0.092538	-0.106
0.22751	0.093618	-0.1007
0.18397	0.162731	-0.2852
-0.8729	-0.18127	0.39916
-0.1091	-0.1544	0.04245
0.16273	0.007448	-0.1863
-0.0392	0.04295	-0.0511
-0.2172	0.00194	0.05043

Dih(C13,C12,C11,C10)	Dih(C12,C11,C10,C9)	Dih(C11,C10,C9,C8)
(179.35) 179.343	(-78.92) -72.597	(-64.36) -64.233
(179.33) 179.316	(-98.50) -102.95	(63.45) 65.629

(179.61) 179.582	(-107.17) -111.5	(64.86) 63.9318
(179.65) 179.61	(-72.34) -68.333	(-64.52) -63.779
(178.35) 179.199	(-88.57) -85.997	(179.87) -177.6
179.313	-103.29	65.0834
179.362	-75.621	-65.317
179.174	-92.437	177.539
179.638	-67.663	-63.486
179.251	-89.548	179.879
179.393	-68.187	-64.149
179.169	-92.005	177.323
179.177	-86.104	-177.26
179.352	-75.699	-65.99
179.385	-71.447	-65.795
179.466	-106.2	67.7428
179.605	-111.47	63.6139
179.261	-89.83	179.888
179.211	-92.307	177.139
179.398	-79.89	-67.749
179.354	-75.893	-65.31
179.161	-86.629	-177.52
179.36	-107.48	66.4673
179.616	-67.971	-63.839
-177.11	-131.47	70.9658
179.667	-112.22	63.5134
179.18	-92.574	177.207
179.247	-88.824	-179.73
179.369	-103.94	65.7888
179.194	-85.97	-179.04
179.179	-86.185	-177.21
179.191	-91.826	176.761
179.393	-70.832	-63.726
179.414	-79.807	-68.068
179.615	-68.319	-74.39
179.098	-90.238	-178.66
179.095	-89.119	178.239
179.16	-87.015	-177.93
179.216	-93.602	178.742

179.734	-111.77	64.4679
179.201	-84.928	-178.74
179.247	-88.915	-179.82
179.358	-103.68	65.967
179.439	-113.48	63.6071
179.199	-85.39	-176.08
179.259	-88.705	-179.92
179.299	-103.27	64.5329
179.347	-75.89	-65.114
179.396	-107.86	65.961
179.103	-89.856	177.678
179.328	-76.624	-65.294
179.643	-68.01	-63.653
179.608	-111.49	63.9246
179.675	-112.36	63.4611
179.638	-67.738	-63.533
179.095	-88.709	178.151
-179.88	-115.57	64.7548
179.174	-84.94	-178.97
179.583	-68.443	-64.047
179.758	-72.32	-71.657
179.196	-86.059	-177.58
179.631	-111.69	63.738
179.167	-86.687	-177.32
179.157	-91.251	177.65
179.473	-65.676	-62.643
179.368	-75.348	-65.791
179.221	-93.795	178.76
179.168	-86.625	-178.41
179.576	-110.43	63.9642
179.261	-88.788	-179.88
179.024	-111.61	65.7274
179.256	-90.344	179.715
-180	-106.4	80.9594
179.103	-111.04	61.5027
179.242	-88.899	-179.81
179.353	-74.954	-65.417

-179.83	-108.22	76.4144
179.586	-111.34	63.3341
179.508	-67.004	-62.729
179.501	-111.01	64.1396
-179.68	-113.89	66.2957
179.339	-103.04	66.3193
179.407	-80.535	-68.191
179.368	-99.321	68.0364
179.406	-79.389	-67.427
179.095	-87.951	178.51
179.392	-108.27	65.6974
-176.38	-41.095	-72.847
179.261	-89.202	-179.99
-177.41	-127.86	68.072
179.226	-94.07	178.683
-179.11	-102.85	87.1144
179.208	-85.05	-178.83
179.162	-86.287	-179.32
-179.34	-104.54	78.0071
-177.57	-149.75	71.4568
179.694	-62.906	-61.402
179.739	-102.86	80.1349
-179.75	-110.09	72.7462
-179.63	-116.41	64.459

Dih(C9,C8,O1,C7)	Dih(C8,O1,C7,C6)	Dih(O1,C7,C6,C5)	Dih(C7,C6,C5,C4)
(-176.81) -177.64	(177.38) -176.31	(62.52) 58.9226	(66.03) 62.1951
(179.42) -178.43	(179.92) 179.425	(59.14) 55.6391	(62.78) 59.7126
(178.79) 178.8	(179.10) -179.32	(59.35) 55.8221	(63.42) 59.6452
(-178.59) -179.06	(179.42) -179.65	(59.71) 55.6494	(63.73) 59.5859
(179.11) 178.13	(178.25) -178.77	(58.62) 54.3296	(61.60) 58.9089
-177.14	179.139	173.714	61.883
177.691	-179.9	173.169	61.8841
179.027	179.596	55.4655	59.6127
-178.59	-179.93	173.362	61.9881

179.622	-179.9	55.6327	59.5747
179.686	75.777	49.2389	60.9028
179.548	179.476	173.263	61.8022
-179.82	179.797	173.231	61.8305
175.682	77.1379	50.7448	60.3972
-81.994	-177.85	56.059	59.843
-178.72	-175.51	-76.713	67.599
176.381	77.2798	50.6894	60.5347
179.724	179.439	173.114	61.7279
-178.68	79.3564	49.5081	60.0915
-79.403	-178.58	55.6119	59.7217
179.112	-178.73	-77.13	65.307
179.297	78.8038	50.5192	60.3831
83.4987	178.817	173.412	61.8934
-178.32	179.486	-77.767	65.1469
-174.91	-178.44	61.153	62.127
179.062	179.617	-77.801	65.2135
177.741	78.6819	167.872	61.4727
178.703	78.5243	50.6624	60.5196
-175.56	-82.358	178.342	63.0774
-79.093	-176.59	55.8471	59.6321
175.967	76.7248	167.582	61.3616
179.01	179.366	-78.979	63.6001
-179.03	-175.68	58.5332	61.3271
-79.461	-178.86	173.291	61.7855
176.95	170.58	51.6045	61.0337
-78.034	-178.48	173.593	61.8167
77.5193	176.964	173.11	61.7537
-177.98	-179.13	-76.877	65.3756
78.2875	175.789	173.089	61.6794
-87.153	178.473	172.893	61.7057
-79.575	-177.24	173.286	61.9954
-179.22	-179.82	-77.468	65.4457
-176.27	-76.835	-69.39	67.319
179.999	-76.355	-66.22	70.0686
-175.86	-77.512	-72.083	65.0692
-179.47	-84.677	177.829	63.0651

-176.48	179.821	176.926	64.3802
177.438	-178.27	175.96	64.5963
82.6193	178.35	-78.038	65.3067
83.1839	83.0403	51.5381	60.4089
179.687	-177.76	-77.805	64.5027
-178.5	-178.7	176.34	64.5993
178.608	179.718	53.1251	57.2323
178.512	-179.54	175.98	64.2767
-178.88	179.658	53.187	57.3206
78.5289	178.067	-77.886	65.3079
170.776	-179.82	172.035	61.5421
-82.509	179.576	-78.556	65.1362
-178.64	179.462	-79.02	64.4616
-175.32	177.956	173.347	61.6951
178.55	-179.99	52.1918	56.9006
179.323	179.836	-78.609	64.8922
-179.55	-178.79	176.23	64.6018
179.084	178.885	53.0138	57.4529
-178.37	77.264	49.0855	59.8612
175.452	76.0689	49.9225	59.2784
78.4885	176.248	-78.193	65.2342
-177.4	-178.4	-77.684	64.2257
176.248	75.2608	48.9625	59.8598
-179.76	-178.8	176.347	64.6749
175.868	-77.89	-67.352	69.9653
179.296	178.934	52.8818	57.1936
-175.4	-175.18	-72.481	69.6705
-174.83	-74.102	103.73	69.0181
-179.24	-179.81	-78.525	64.8819
170.723	73.2689	168.822	62.3306
-179.99	81.7121	50.6583	60.1179
172.043	73.8263	168.786	62.2444
-178.05	82.3714	171.71	63.6448
-179.23	-82.669	-178.67	66.1044
165.369	71.5977	168.091	61.432
179.01	-82.926	-73.177	66.5327
-78.518	-177.48	176.43	64.378

79.7484	179.819	176.291	64.6457
-80.05	179.961	52.9982	57.6181
78.8793	179.628	176.191	64.6704
82.3996	178.335	-79.055	65.0206
169.669	179.604	-85.9	64.8649
-177.84	-81.768	-178.88	66.1571
179.878	176.753	55.283	58.4319
79.2893	177.624	175.976	64.1913
-75.463	-174.34	173.919	63.4017
-79.369	-177.58	53.3786	57.4268
-83.2	179.397	-79.712	64.8181
178.512	-178.66	-79.31	62.6954
-164.52	-70.299	-74.574	64.4567
-163.5	179.383	-179.97	65.5011
179.242	-175.99	177.213	65.6875
175.952	76.9537	48.7698	59.1203
163.205	69.9935	168.922	61.9013

Dih(C6,C5,C4,C3)		Dih(C5,C4,C3,C2)		Dih(C4,C3,C2,C1)		Dih(C3,C2,C1,N1)	
(175.30)	175.551	(-53.24)	-52.433	(52.77)	52.1269	(-56.00)	-55.857
(175.11)	175.382	(-53.06)	-52.278	(52.78)	52.2042	(-56.09)	-55.958
(175.15)	175.383	(-53.08)	-52.266	(52.78)	52.2027	(-56.08)	-55.98
(175.15)	175.406	(-53.09)	-52.267	(52.79)	52.1831	(-56.10)	-55.959
(175.09)	175.543	(-53.01)	-52.296	(52.79)	52.2047	(-56.10)	-55.937
	175.817		-52.268		52.1125		-55.659
	175.863		-52.277		52.1164		-55.648
	175.393		-52.28		52.201		-55.953
	175.884		-52.271		52.1082		-55.646
	175.385		-52.266		52.1894		-55.975
	175.479		-52.356		52.2512		-55.931
	175.855		-52.275		52.111		-55.641
	175.86		-52.276		52.1123		-55.638
	175.367		-52.361		52.282		-55.915
	175.354		-52.264		52.1972		-55.979
	175.251		-52.285		52.3099		-55.95

175.371	-52.367	52.2866	-55.918
175.892	-52.271	52.0968	-55.63
175.589	-52.401	52.2818	-55.886
175.363	-52.278	52.2017	-55.962
174.788	-51.992	52.4505	-56.185
175.365	-52.367	52.2923	-55.928
175.886	-52.267	52.1108	-55.652
174.897	-51.998	52.4449	-56.179
174.018	-51.197	51.715	-56.473
174.922	-52.008	52.4349	-56.149
175.636	-52.309	52.1741	-55.713
175.344	-52.37	52.2983	-55.935
175.624	-52.305	52.2197	-55.727
175.376	-52.266	52.1812	-55.956
175.664	-52.308	52.1659	-55.704
174.757	-51.885	52.4873	-56.229
71.6913	53.4103	-52.196	53.7264
175.819	-52.264	52.1113	-55.653
175.953	-52.261	52.0705	-56.056
175.799	-52.258	52.1115	-55.658
175.87	-52.274	52.1128	-55.638
174.761	-51.982	52.4544	-56.192
175.884	-52.262	52.0971	-55.651
175.879	-52.259	52.0907	-55.64
175.856	-52.267	52.1148	-55.647
174.853	-52.012	52.4615	-56.163
174.373	-52.029	52.4006	-56.255
174.243	-52.074	52.3972	-56.276
174.187	-51.882	52.4638	-56.354
175.638	-52.318	52.2333	-55.71
71.3964	52.7925	-51.71	54.002
71.5679	52.6898	-51.722	54.0927
174.928	-52.02	52.4349	-56.158
175.294	-52.348	52.287	-55.946
70.2568	53.5753	-51.633	53.5589
71.5363	52.6993	-51.697	54.0851
71.6086	53.5828	-52.436	53.8234

71.5446	52.7415	-51.725	54.0624
71.6121	53.5715	-52.424	53.8197
174.876	-52.027	52.4485	-56.147
176.066	-52.24	52.0163	-55.606
174.983	-52.035	52.4374	-56.147
70.5394	53.4461	-51.672	53.6926
176.014	-52.234	52.0238	-55.614
71.6694	53.591	-52.465	53.8142
70.4955	53.413	-51.626	53.6943
71.5579	52.6954	-51.715	54.0822
71.6328	53.5499	-52.434	53.8307
71.8602	53.4558	-52.351	53.71
71.8908	53.5835	-52.453	53.6909
174.952	-52.028	52.4314	-56.126
70.2251	53.6098	-51.625	53.529
71.7215	53.1492	-52.277	54.042
71.5484	52.6842	-51.693	54.0824
70.2768	53.2544	-51.563	53.8918
71.6524	53.5858	-52.469	53.8241
174.561	-52.092	52.4809	-56.283
176.331	-52.793	51.9149	-55.353
70.4895	53.4195	-51.637	53.6955
71.7132	52.9562	-51.993	53.9627
175.356	-52.332	52.3058	-55.996
71.6936	52.9869	-52.005	53.9476
71.4787	52.8748	-51.825	53.9444
71.4188	52.6031	-51.636	54.1464
175.666	-52.293	52.1598	-55.738
70.4685	53.4799	-51.746	53.6902
71.4315	52.7773	-51.713	54.0153
71.557	52.6872	-51.712	54.087
71.6246	53.5349	-52.428	53.8399
71.5649	52.6821	-51.711	54.0884
70.5834	53.3777	-51.658	53.7433
175.924	-52.567	52.5859	-55.867
71.471	52.601	-51.703	54.1821
71.2323	53.7442	-52.414	53.7457

71.5459	52.7534	-51.735	54.0527
71.777	52.6646	-51.735	54.1808
71.6052	53.5662	-52.421	53.8161
70.6412	53.3678	-51.678	53.7533
70.3018	53.6521	-51.637	53.5346
174.421	-51.82	52.4358	-56.366
71.0582	52.661	-51.438	53.9827
71.4912	52.5244	-51.545	54.136
71.6939	53.2571	-52.336	54.008
71.6937	53.0309	-52.029	53.9332

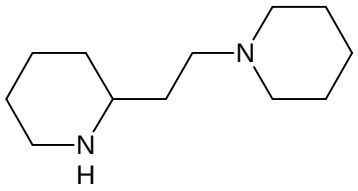
Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,C7)
(62.12) 59.8175	(176.14) 178.291	(-174.09) -176.46
(62.18) 59.6732	(176.01) 178.346	(-177.19) -178.66
(62.13) 59.6927	(176.03) 178.321	(-176.52) -178.72
(62.17) 59.7157	(176.04) 178.278	(-176.26) -178.8
(62.11) 59.6439	(175.99) 178.206	(-178.26) -179.36
59.5787	177.988	-176.28
59.5544	177.977	-176.25
59.6753	178.327	-178.76
59.5688	177.947	-176.14
59.7183	178.302	-178.81
59.5294	178.52	-177.43
59.5618	177.966	-176.34
59.5565	177.967	-176.31
59.4788	178.592	-177.94
59.7079	178.339	-178.55
59.4878	178.188	-170.51
59.4708	178.609	-177.8
59.578	177.914	-176.41
59.4437	178.44	-178.14
59.682	178.351	-178.67
59.441	178.32	-172.52
59.4704	178.614	-177.95
59.5666	177.94	-176.22

59.4284	178.259	-172.62
60.4662	178.831	-176.59
59.426	178.242	-172.57
59.5094	178.266	-176.77
59.4641	178.645	-177.82
59.4639	178.25	-175.08
59.7208	178.297	-178.77
59.5165	178.234	-176.88
59.326	178.41	-174.02
-56.356	-71.927	-173.49
59.577	177.972	-176.37
59.939	177.865	-177.26
59.5834	177.984	-176.35
59.5512	177.956	-176.37
59.4399	178.336	-172.45
59.5946	177.909	-176.45
59.6021	177.892	-176.44
59.5601	177.964	-176.13
59.3893	178.332	-172.34
59.6974	178.397	-170.94
59.7866	178.55	-168.4
59.5484	178.642	-172.98
59.4182	178.292	-175.07
-56.863	-71.582	-170.13
-56.921	-71.646	-169.84
59.433	178.245	-172.49
59.5057	178.615	-177.96
-56.527	-72.203	-169.85
-56.963	-71.591	-169.85
-55.641	-73.072	-176.99
-56.911	-71.649	-170.17
-55.667	-73.03	-176.92
59.403	178.304	-172.5
59.6893	177.651	-176.57
59.4058	178.241	-172.63
-56.596	-72.3	-169.78
59.705	177.701	-176.45

-55.592	-73.153	-177.26
-56.671	-72.191	-169.4
-56.932	-71.632	-169.85
-55.649	-73.06	-176.78
-56.011	-72.323	-174.73
-55.83	-72.629	-175.22
59.4121	178.237	-172.55
-56.499	-72.238	-170.11
-55.952	-72.786	-174.39
-56.972	-71.578	-169.79
-57.009	-72.034	-164.89
-55.594	-73.14	-177.03
59.5144	178.624	-168.44
59.8603	177.913	-169.96
-56.647	-72.23	-169.39
-56.365	-72.273	-171.99
59.4903	178.578	-178.16
-56.33	-72.295	-172.08
-56.617	-71.797	-170.86
-57.097	-71.506	-168.44
59.5551	178.204	-176.81
-56.511	-72.428	-167.96
-56.882	-71.599	-170.11
-56.935	-71.627	-169.8
-55.657	-73.041	-176.63
-56.939	-71.625	-169.77
-56.671	-72.241	-169.26
58.9819	178.186	-172.73
-56.994	-71.683	-168.33
-55.569	-72.838	-176.07
-56.889	-71.675	-170.25
-57.038	-71.822	-170.82
-55.667	-73.022	-176.83
-56.638	-72.302	-169.41
-56.518	-72.288	-171.44
59.479	178.518	-173.36
-57.214	-70.936	-169.23

-57.221	-71.212	-168.85
-55.835	-72.931	-175.07
-56.301	-72.341	-172.41

Compound 37



Molecule (-577.2831138 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	-2.1283	0	-0.0034	0
Conformer.2	-0.5993	1.52895	-0.001	0.00244
Conformer.3	0.2669	2.39516	0.00043	0.00382
Conformer.4	1.24898	3.37723	0.00199	0.00538
Conformer.5	2.01631	4.14456	0.00321	0.0066
Conformer.6	2.55518	4.68344	0.00407	0.00746
Conformer.7	2.6231	4.75135	0.00418	0.00757
Conformer.8	3.76387	5.89212	0.006	0.00939
Conformer.9	5.2089	7.33715	0.0083	0.01169
Conformer.10	6.16247	8.29072	0.00982	0.01321
Conformer.11	6.30253	8.43078	0.01004	0.01344

Conformation Energy	Relative energy
-577.2840445	0
-577.2831138	0.000931
-577.2820445	0.002
-577.2786723	0.005372
-577.2777405	0.006304

Dih(N2,C8,C12,C10)	Dih(C8,C12,C10,C11)	Dih(C12,C10,C11,C9)
-55.911	52.4012	-52.473
-56.277	52.5584	-52.449
-56.214	52.4624	-52.398
53.7921	-51.057	51.2495
-56.339	52.6573	-52.466
54.4386	-51.163	50.8301
-56.165	52.1766	-52.287
54.0474	-51.192	51.0703
54.095	-50.957	50.9395
54.5443	-51.567	50.9415
-56.176	52.8342	-52.551

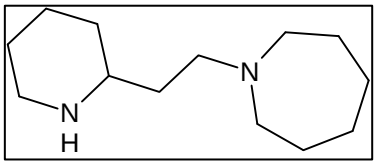
Dih(C11,C9,N2,C7)	Dih(C9,N2,C7,C4)	Dih(N2,C7,C4,C3)	Dih(C7,C4,C3,C5)
177.045	-168.39	53.3369	59.3079
178.904	-71.228	179.641	64.0503
178.041	-67.389	-68.158	72.1874
-73.29	-167.27	53.3992	59.3854
179.177	-68.24	-176.49	67.6891
-71.696	-70.095	179.626	63.8754
177.579	-71.83	-70.303	73.639
-72.442	-65.996	-68.509	72.1843
-71.416	-67.154	-176.6	67.3823
-72.751	-70.123	-70.065	74.4801
178.957	-65.168	104.664	69.0983

Dih(C4,C3,C5,C1)	Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)	Dih(C1,C6,C2,N1)
175.478	-52.353	52.2318	-55.968
175.66	-52.257	52.1495	-55.76
174.545	-52.202	52.3062	-56.214
175.442	-52.35	52.2303	-55.967
71.2623	52.5499	-51.49	54.1797
175.672	-52.248	52.1508	-55.767
70.6667	52.9329	-51.535	54.2212
174.57	-52.207	52.2958	-56.202
71.2531	52.5904	-51.505	54.1563

70.687	52.8605	-51.516	54.2706
72.3616	51.7008	-51.506	54.7467

Dih(C6,C2,N1,C3)	Dih(C2,N1,C3,C4)	Dih(N1,C3,C4,C7)
59.6355	178.312	-179.05
59.685	177.901	-174.15
59.9589	178.051	-166.36
59.6421	178.334	-178.99
-57.358	-71.311	-166.97
59.6824	177.888	-174.3
-57.449	-71.969	-161.17
59.966	178.021	-166.36
-57.316	-71.35	-167.26
-57.539	-71.849	-160.39
-57.743	-71.141	-165.81

Compound 38



Molecule (-616.3021957 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	8.88589	0	0.01416	0
Conformer.2	9.36487	0.47897	0.01492	0.00076
Conformer.3	9.5005	0.61461	0.01514	0.00098
Conformer.4	9.60396	0.71807	0.0153	0.00114
Conformer.5	9.72342	0.83752	0.0155	0.00133
Conformer.6	9.74048	0.85459	0.01552	0.00136
Conformer.7	9.83953	0.95364	0.01568	0.00152
Conformer.8	9.83972	0.95383	0.01568	0.00152
Conformer.9	9.9408	1.05491	0.01584	0.00168

Conformer.10	9.95236	1.06647	0.01586	0.0017
Conformer.11	9.95879	1.0729	0.01587	0.00171
Conformer.12	9.97845	1.09255	0.0159	0.00174
Conformer.13	9.99427	1.10838	0.01593	0.00177
Conformer.14	10.1626	1.27675	0.0162	0.00203
Conformer.15	10.1763	1.29043	0.01622	0.00206
Conformer.16	10.3087	1.42285	0.01643	0.00227
Conformer.17	10.3348	1.44895	0.01647	0.00231
Conformer.18	10.4311	1.54518	0.01662	0.00246
Conformer.19	10.6734	1.78747	0.01701	0.00285
Conformer.20	10.8096	1.92371	0.01723	0.00307
Conformer.21	10.813	1.92712	0.01723	0.00307
Conformer.22	10.8272	1.94126	0.01725	0.00309
Conformer.23	10.8858	1.99988	0.01735	0.00319
Conformer.24	10.9159	2.02997	0.0174	0.00323
Conformer.25	10.9325	2.04663	0.01742	0.00326
Conformer.26	11.1514	2.26555	0.01777	0.00361
Conformer.27	11.1724	2.28653	0.0178	0.00364
Conformer.28	11.2387	2.35283	0.01791	0.00375
Conformer.29	11.25	2.36407	0.01793	0.00377
Conformer.30	11.3424	2.45656	0.01808	0.00391
Conformer.31	11.3697	2.48384	0.01812	0.00396
Conformer.32	11.5366	2.65074	0.01838	0.00422
Conformer.33	11.545	2.65911	0.0184	0.00424
Conformer.34	11.5533	2.66736	0.01841	0.00425
Conformer.35	11.5843	2.6984	0.01846	0.0043
Conformer.36	11.5969	2.71098	0.01848	0.00432
Conformer.37	11.6563	2.77038	0.01858	0.00441
Conformer.38	11.6796	2.79369	0.01861	0.00445
Conformer.39	11.7081	2.82218	0.01866	0.0045
Conformer.40	11.7546	2.86868	0.01873	0.00457
Conformer.41	11.7622	2.87631	0.01874	0.00458
Conformer.42	11.8134	2.92754	0.01883	0.00467
Conformer.43	11.8253	2.93944	0.01884	0.00468
Conformer.44	11.8479	2.96199	0.01888	0.00472
Conformer.45	12.0879	3.20205	0.01926	0.0051
Conformer.46	12.0954	3.20955	0.01928	0.00511

Conformer.47	12.1366	3.2507	0.01934	0.00518
Conformer.48	12.3112	3.42529	0.01962	0.00546
Conformer.49	12.4439	3.558	0.01983	0.00567
Conformer.50	12.5288	3.64288	0.01997	0.00581
Conformer.51	12.5463	3.66042	0.01999	0.00583
Conformer.52	12.793	3.90712	0.02039	0.00623
Conformer.53	12.8168	3.93088	0.02042	0.00626
Conformer.54	12.8624	3.97649	0.0205	0.00634
Conformer.55	12.9961	4.1102	0.02071	0.00655
Conformer.56	13.0011	4.11525	0.02072	0.00656
Conformer.57	13.0896	4.20374	0.02086	0.0067
Conformer.58	13.2072	4.32129	0.02105	0.00689
Conformer.59	13.2181	4.33218	0.02106	0.0069
Conformer.60	13.2349	4.34899	0.02109	0.00693
Conformer.61	13.3381	4.4522	0.02126	0.0071
Conformer.62	13.4536	4.56771	0.02144	0.00728
Conformer.63	13.5064	4.62055	0.02152	0.00736
Conformer.64	13.5561	4.67022	0.0216	0.00744
Conformer.65	13.5928	4.70688	0.02166	0.0075
Conformer.66	13.6121	4.7262	0.02169	0.00753
Conformer.67	13.6182	4.73229	0.0217	0.00754
Conformer.68	13.6219	4.73602	0.02171	0.00755
Conformer.69	13.8034	4.91746	0.022	0.00784
Conformer.70	13.8663	4.98038	0.0221	0.00794
Conformer.71	13.8855	4.99958	0.02213	0.00797
Conformer.72	13.8858	4.99988	0.02213	0.00797
Conformer.73	13.9124	5.02648	0.02217	0.00801
Conformer.74	13.9191	5.03316	0.02218	0.00802
Conformer.75	13.9485	5.0626	0.02223	0.00807
Conformer.76	14.0305	5.14465	0.02236	0.0082
Conformer.77	14.0582	5.17226	0.0224	0.00824
Conformer.78	14.1519	5.26597	0.02255	0.00839
Conformer.79	14.1831	5.29719	0.0226	0.00844
Conformer.80	14.2199	5.33405	0.02266	0.0085
Conformer.81	14.3307	5.44481	0.02284	0.00868
Conformer.82	14.5495	5.66361	0.02319	0.00903
Conformer.83	15.0601	6.17421	0.024	0.00984

Conformer.84	15.1534	6.26746	0.02415	0.00999
Conformer.85	15.3028	6.41694	0.02439	0.01023
Conformer.86	15.3551	6.46916	0.02447	0.01031
Conformer.87	15.5502	6.66427	0.02478	0.01062
Conformer.88	15.678	6.79209	0.02498	0.01082
Conformer.89	15.7348	6.84893	0.02508	0.01091
Conformer.90	15.7823	6.89643	0.02515	0.01099
Conformer.91	15.8414	6.95548	0.02524	0.01108
Conformer.92	15.8437	6.95782	0.02525	0.01109
Conformer.93	16.6686	7.78269	0.02656	0.0124
Conformer.94	16.6762	7.79033	0.02658	0.01241
Conformer.95	16.7132	7.82729	0.02663	0.01247
Conformer.96	17.0379	8.15203	0.02715	0.01299
Conformer.97	17.1333	8.2474	0.0273	0.01314
Conformer.98	17.4916	8.60572	0.02787	0.01371
Conformer.99	17.5162	8.63035	0.02791	0.01375
Conformer.100	17.5693	8.68342	0.028	0.01384

Conformation Energies	Relative Energies
-616.3054362	0.001925
-616.3037768	0.003584
-616.3052066	0.002154
-616.307361	0
-616.3063434	0.001018

Dih(N2,C8,C12,C10)	Dih(C8,C12,C10,C11)	Dih(C12,C10,C11,C9)
(39.11) 40.5186	(-85.72) -85.702	(66.33) 68.0585
(-87.88) -88.391	(37.49) 37.0025	(35.33) 37.8176
(71.37) 75.4144	(-49.20) -53.58	(66.49) 67.8929
(72.70) 74.5366	(-50.09) -52.81	(65.71) 68.1691
(-71.33) -74.812	(49.32) 53.092	(-66.57) -68.077
-57.381	72.4035	-81.326
73.6373	-52.555	68.6526
-75.426	53.5306	-67.876

73.8992	-52.536	68.4774
-74.358	83.7629	-37.541
74.605	-83.645	36.8704
-45.535	-33.522	82.1158
-72.28	51.9787	-69.298
-88.699	37.594	37.5178
-88.535	37.1737	37.6635
47.8943	31.4069	-81.466
-74.05	83.604	-38.053
37.7182	-84.996	68.4399
-59.91	76.596	-77.566
59.5647	-76.162	77.7155
-88.114	68.499	-54.176
73.8452	-83.647	38.4235
-59.677	76.4219	-77.659
88.3996	-36.206	-38.44
48.5326	30.7995	-81.222
-48.836	-24.843	77.4615
-85.311	72.2625	-54.444
-49.386	-24.45	77.4785
86.789	-35.989	-38.365
37.5721	-85.207	68.7631
-73.541	83.7033	-38.309
-48.928	-24.707	77.5671
-60.092	76.2755	-77.457
74.2368	-83.642	37.6105
-41.779	85.7647	-67.858
59.695	-76.448	77.6141
88.0784	-68.555	54.1352
37.3894	-84.947	68.4787
50.5602	-54.385	-29.579
-88.718	37.5797	37.5314
49.3835	24.1621	-77.309
59.124	-76.195	77.7971
73.5654	-52.254	68.5576
-38.295	85.4269	-69.6
88.4345	-36.503	-38.126

-89.042	37.9376	37.4214
-56.887	72.1533	-81.207
40.5047	-85.709	68.0783
45.4341	-59.296	-22.152
-87.052	69.8119	-53.654
-1.8516	-68.593	29.4736
0.22893	68.8087	-27.915
74.3483	-53.349	67.523
59.6911	-76.417	77.6379
-40.751	85.7097	-68.023
-55.2	-32.714	66.4109
86.713	-36.163	-38.288
48.8092	24.833	-77.389
-73.971	52.6191	-68.413
-49.337	86.589	-67.483
55.26	32.6662	-66.414
-86.782	36.3124	38.1384
88.4354	-37.222	-37.653
-48.995	-24.916	77.6922
39.5928	-85.162	69.0157
-89.241	38.108	37.5279
-69.795	-1.7821	67.219
55.3776	32.8629	-66.157
37.848	-85.014	68.4911
-54.531	-33.7	65.9758
57.3495	-72.483	81.257
-48.922	-26.005	78.6712
88.3054	-36.349	-38.288
48.9417	-86.829	67.5114
-57.106	-30.132	67.1877
-60.523	76.8976	-77.319
-57.447	72.1942	-81.795
-1.7866	-68.232	28.9484
48.8874	24.9844	-77.745
-88.07	68.5629	-54.15
-70.181	1.63978	66.2708
-51.95	52.4256	30.9108

55.0802	32.8983	-66.334
50.6849	-54.269	-29.727
87.6236	-70.446	53.7431
87.7077	-69.732	55.8017
-74.206	53.1308	-67.525
-70.304	1.76616	66.2193
-54.497	-33.725	65.973
67.6348	11.8834	-69.068
64.0316	8.10421	-69.106
-50.989	53.9875	30.0891
70.6817	-7.7982	-64.174
69.9291	-0.727	-66.61
-8.1946	71.5552	-24.439
-58.165	-12.899	73.371
82.0855	-30.269	-41.794
-63.317	-10.247	69.625
54.7001	33.3495	-66.15
-48.923	86.6177	-67.515

Dih(C11,C9,C13,N2)	Dih(C9,C13,N2,C7)	Dih(C13,N2,C7,C4)	Dih(N2,C7,C4,C3)
(71.73) 74.8445	(136.09) 141.771	(-163.67) -168.70	(54.15) 54.6397
(73.27) 73.9725	(173.07) 174.608	(-159.63) -161.73	(52.53) 51.9486
(38.50) 41.8112	(175.43) 165.628	(63.64) 59.78	(163.13) 168.715
(40.48) 39.3844	(170.77) 168.532	(64.87) 66.60	(66.05) 63.7312
(-38.17) -40.401	(-175.15) -167.58	(-64.31) -62.841	(-50.77) -54.286
47.7101	144.489	-166.740854	51.2248
37.6626	171.477	159.53702	-53.382
-41.689	-165.13	-61.5592715	-171.09
37.4733	171.172	156.737575	-173.96
88.5048	158.688	-164.71587	60.7141

-88.442	-160.43	73.3484763	60.305
57.466	163.132	-163.27316	61.5548
-37.019	-169.7	-157.35254	65.1552
73.852	176.873	-66.4147555	-51.797
74.0629	174.942	-160.520017	168.344
-56.784	-162.46	164.782332	-51.387
88.4562	159.232	-77.5302392	-172.6
73.9509	141.106	-74.7924808	-171.52
48.9189	49.7231	62.9627413	56.0843
-48.977	-50.145	-163.058168	54.5746
-85.68	164.218	62.1757571	55.9728
-88.369	-158.7	80.5415752	-177.48
48.992	49.5635	61.5442639	170.895
-73.788	-174.71	154.634025	175.557
-56.853	-163.15	162.247527	-171.5
60.1402	64.8943	61.5667947	168.599
-88.04	-86.077	-168.607004	169.315
59.7087	66.6333	164.254653	-173.15
-73.708	-169.5	-66.5929799	-174.73
73.3478	141.676	-74.4762223	-74.66
86.7216	153.258	62.9023871	-175.8
59.8957	66.9424	164.12865	-56.052
48.8956	49.7894	163.762874	-170.95

-88.469	-159.27	78.2939953	65.1713
-75.472	-143.36	170.994676	-170.81
-49.087	-49.415	-61.9301741	-171.5
85.8222	-164.37	-61.4958531	-55.888
73.8716	141.595	-76.5411486	-173.95
1.92343	156.696	-168.693741	54.3706
73.8452	176.353	-66.4043264	-67.467
-60.125	-66.226	-162.757888	66.0041
-49.473	-49.402	-161.118817	63.4881
37.3413	171.015	74.0196263	68.3129
-73.556	-146.93	79.4135111	68.0953
-74.043	-175.25	157.31567	-172.61
73.639	178.347	-67.3790977	-169.4
48.5828	145.497	-77.9702493	-174.22
74.8431	141.948	-169.722355	53.7367
-8.2175	162.528	-167.058053	63.0304
-87.73	170.003	155.445324	-170.06
-50.45	-166.52	-63.6761532	-53.92
48.724	169.859	162.613686	-49.94
49.5515	-112.18	-168.655622	170.063
-48.978	-48.999	-62.5248736	-171.95
-74.945	-141.7	169.53262	-54.935
-70.071	160.052	61.1655259	169.882

-73.565	-169.51	-67.902721	-175.8
-60.267	-64.178	-63.0915805	-170.86
-37.89	-171.72	-156.753865	173.548
-74.242	-54.504	-55.0892373	-172.03
70.1578	-159.48	-63.1025384	-172.31
73.7106	169.504	69.0876087	-177.05
-73.983	-174.51	163.078413	-50.93
59.6343	66.9658	164.529319	-172.25
73.5367	137.287	62.7708679	-173.55
73.2149	178.551	-64.2866404	-174.5
-57.425	-74.019	-162.960262	65.15
70.1761	-160.76	-166.605383	167.461
73.7892	140.664	-76.9447575	-66.261
-70.251	158.365	63.8224	-179.89
-47.918	-144.37	168.215745	-49.983
57.9931	66.3435	73.2091017	67.9464
-73.898	-174.23	159.23053	-70.546
73.4594	54.0869	59.0753647	67.5339
-69.797	163.877	164.723848	-52.476
49.0293	48.8353	71.1565508	70.3147
46.397	146.692	-76.6016523	-70.682
-51.138	-164.75	-61.3350688	-72.661
-59.56	-67.215	-164.983447	172.236

-85.789	164.477	61.2968031	54.9973
-55.575	-71.828	-62.0727649	-168
-7.9391	-158.37	76.1478863	68.4722
70.2217	-159.18	-62.9889044	-172.1
2.24313	156.755	-169.875162	53.5148
86.9611	90.1604	73.7703499	171.935
82.486	105.782	-65.7658513	176.087
-49.035	111.516	168.255468	-171.54
-55.536	-71.154	-63.3318356	-169.84
-70.238	158.357	63.8731262	-179.15
61.412	81.6316	75.312033	65.5105
60.7068	169.624	70.837335	-174.6
-2.7305	-156.33	169.68033	-54.751
51.954	70.4962	157.631879	82.8619
55.8096	73.8394	165.120926	-56.562
46.5911	176.594	-74.2771036	174.983
55.9492	89.592	-53.2515053	-172.19
-71.834	-75.799	-74.6350487	-64.68
-61.408	-170.37	-72.1181381	173.576
70.0369	-159.16	-63.6836081	-65.047
-73.922	-55.131	-54.9584269	-64.487

Dih(C7,C4,C3,C5) Dih(C4,C3,C5,C1) Dih(C3,C5,C1,C6) Dih(C5,C1,C6,C2)

(60.62) 59.2672	(175.06) 175.441	(-52.95) -52.328	(52.71) 52.2472
(58.92) 59.1154	(174.89) 175.567	(-52.85) -52.379	(52.74) 52.2183
(64.03) 61.6947	(175.42) 175.748	(-52.88) -52.256	(52.71) 52.1167
(167.50) 167.672	(177.42) 179.313	(-52.75) -52.228	(52.47) 50.8705
(-174.82) 177.572	(176.74) 177.979	(-53.26) -52.744	(53.22) 52.3495
58.9403	175.595	-52.382	52.2293
178.019	178.065	-52.742	52.3389
174.449	178.09	-52.357	51.7572
174.208	178.032	-52.378	51.7958
167.19	179.108	-52.25	50.9069
166.742	178.911	-52.254	50.8961
166.596	178.974	-52.223	50.8031
166.864	179.126	-52.205	50.7598
178.352	177.974	-52.721	52.3425
61.7759	175.83	-52.257	52.0918
178.751	178.088	-52.713	52.3251
174.335	178.049	-52.372	51.7845
172.287	178.12	-52.901	52.3667
59.5617	175.357	-52.309	52.232
59.4476	175.418	-52.333	52.2305
59.6407	175.352	-52.317	52.2417
175.422	178.102	-52.44	51.9609
62.4617	175.644	-52.226	52.1113
62.6087	175.763	-52.229	52.1363
172.353	178.098	-52.906	52.3843
61.7658	175.716	-52.231	52.12
61.8063	175.727	-52.251	52.1204
174.236	178.008	-52.387	51.8035
171.051	178.118	-52.909	52.2887
70.0355	174.974	-52.265	52.321
173.827	178.107	-52.369	51.7604
176.665	177.906	-52.778	52.3563
174.518	178.066	-52.375	51.7907
167.068	75.9133	52.7035	-53.325
175.363	74.4276	51.6173	-51.802
171.933	178.114	-52.903	52.3374
176.73	177.871	-52.777	52.3712

175.215	74.338	51.552	-51.712
59.1371	175.504	-52.345	52.2449
72.3206	174.629	-52.248	52.2984
167.372	179.346	-52.246	50.8865
167.171	179.238	-52.256	50.9125
166.045	77.0024	52.9494	-53.94
163.8	76.1121	52.853	-53.724
175.326	74.3924	51.5415	-51.731
175.513	74.4787	51.5864	-51.805
175.139	74.335	51.5536	-51.721
57.9201	71.6531	53.3557	-52.305
167.048	179.18	-52.238	50.8654
172.502	178.119	-52.898	52.3652
177.839	178.034	-52.73	52.3312
179.564	178.206	-52.676	52.2801
62.3292	175.644	-52.24	52.1281
175.398	74.4498	51.6294	-51.788
178.269	74.407	51.6409	-51.269
61.8736	175.727	-52.245	52.1152
174.697	74.3135	51.7176	-51.778
175.792	74.3494	51.5609	-51.695
64.2706	71.5054	52.8851	-51.76
174.389	178.016	-52.381	51.7987
174.399	178.078	-52.366	51.7727
171.875	74.2909	52.3699	-51.721
179.343	74.4981	51.528	-51.25
172.249	74.4123	52.292	-51.786
172.309	74.3885	52.3129	-51.742
68.557	71.2406	52.4941	-51.467
167.278	179.295	-52.247	50.8823
61.6059	175.771	-52.256	52.1188
169.776	74.0264	52.5838	-52.462
175.075	178.06	-52.45	51.9787
179.89	74.5682	51.4607	-51.221
165.891	76.6145	52.9321	-53.77
71.8278	69.8533	53.5119	-51.522
168.37	179.493	-52.254	50.9595

177.964	177.937	-52.736	52.3454
164.573	77.0921	53.046	-54.115
76.4845	70.8465	52.8307	-51.739
69.2652	174.898	-52.244	52.3335
63.4214	71.4074	52.98	-51.782
58.3364	71.6179	53.3284	-52.275
172.873	178.106	-52.891	52.3666
167.745	75.8374	52.5972	-53.216
175.446	74.3796	51.5969	-51.754
57.7862	71.6727	53.3633	-52.318
63.6821	71.5422	52.9302	-51.795
65.1554	71.3667	52.8432	-51.771
172.304	74.408	52.2787	-51.791
175.767	74.4012	51.5556	-51.732
176.039	74.3095	51.5633	-51.514
167.161	76.0656	52.7495	-53.386
171.222	178.143	-52.902	52.2795
178.39	74.4153	51.6206	-51.26
57.8882	175.186	-52.414	52.1553
177.529	74.3204	51.7274	-51.307
64.2247	71.4161	52.9115	-51.823
171.806	178.239	-52.872	52.2602
170.188	74.0487	52.5466	-52.43
63.026	71.7003	53.4108	-52.113
169.609	74.0493	52.5943	-52.498
169.358	74.0416	52.6268	-52.5

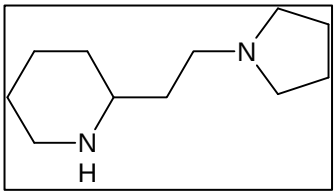
Dih(C1,C6,C2,N1)	Dih(C6,C2,N1,C3)	Dih(C2,N1,C3,C4)	Dih(N1,C3,C4,C7)
(-56.07) -55.977	(62.18) 59.6129	(176.09) 178.305	(-179.33) -179.04
(-56.16) -55.949	(62.19) 59.6497	(176.11) 178.238	(179.04) -179.24
(-56.01) -55.735	(62.04) 59.6499	(175.92) 177.985	(-175.56) -176.52
(-56.03) -54.757	(61.96) 60.9389	(176.95) 175.919	(-71.61) -70.864
(-56.55) -55.839	(61.26) 59.2715	(178.93) -179.9	(-54.16) -60.522
-55.951	59.6253	178.22	-179.38
-55.858	59.3128	-179.99	-60.049
-55.439	59.2753	178.928	-63.237
-55.443	59.2147	179.024	-63.471

-54.814	60.9305	176.069	-71.441
-54.796	60.9367	176.101	-71.994
-54.709	61.0219	175.847	-72.173
-54.623	61.0016	175.716	-71.825
-55.847	59.286	-179.96	-59.713
-55.706	59.6695	177.929	-176.43
-55.863	59.3348	179.925	-59.279
-55.444	59.2303	178.985	-63.34
-55.546	58.9609	-179.81	-65.759
-55.985	59.661	178.327	-178.81
-55.964	59.6389	178.335	-178.92
-55.984	59.638	178.37	-178.73
-55.448	58.9849	179.389	-62.092
-55.763	59.7052	178.031	-175.81
-55.746	59.6655	177.808	-175.49
-55.56	58.9417	-179.77	-65.688
-55.757	59.6691	177.986	-176.44
-55.741	59.6508	177.997	-176.41
-55.441	59.2185	179.065	-63.472
-55.475	59.0744	-179.91	-67.139
-56.101	59.7263	177.938	-168.21
-55.394	59.2863	178.958	-63.889
-55.828	59.2703	-179.78	-61.523
-55.442	59.2341	179.011	-63.163
55.2685	-55.936	-73.831	-66.071
54.8656	-57.13	-71.292	-58.432
-55.533	59.0167	-179.85	-66.177
-55.835	59.2443	-179.75	-61.445
54.8844	-57.282	-71.092	-58.621
-55.966	59.6066	178.261	-179.15
-56.182	59.9507	177.992	-166.23
-54.764	60.9143	176.002	-71.16
-54.808	60.9129	176.083	-71.403
55.4373	-55.165	-75.472	-66.507
55.6018	-55.701	-74.57	-69.152
54.8996	-57.254	-71.174	-58.484
54.8906	-57.13	-71.351	-58.255

54.889	-57.265	-71.118	-58.698
53.9287	-55.83	-73.026	-176.28
-54.757	60.9641	175.963	-71.582
-55.543	58.9599	-179.83	-65.539
-55.838	59.2978	-179.98	-60.23
-55.841	59.3765	179.718	-58.394
-55.763	59.6676	178.077	-175.93
54.8663	-57.185	-71.228	-58.393
54.3209	-58.189	-69.055	-56.493
-55.742	59.6637	177.98	-176.34
54.7364	-57.14	-71.111	-59.198
54.8388	-57.275	-71.043	-58.066
53.9488	-56.739	-71.747	-170.21
-55.44	59.2236	179.052	-63.314
-55.439	59.2541	178.966	-63.283
54.1391	-57.349	-70.005	-62.554
54.4073	-58.286	-69.104	-55.366
54.2726	-57.306	-70.228	-62.092
54.1895	-57.332	-70.13	-62.061
54.2225	-57.436	-71.252	-166.17
-54.757	60.9146	175.998	-71.278
-55.733	59.6429	177.998	-176.6
54.5348	-56.053	-71.934	-64.464
-55.438	58.9564	179.462	-62.455
54.4385	-58.354	-69.087	-54.785
55.3723	-55.361	-74.979	-66.839
53.733	-57.016	-71.768	-163.1
-54.791	60.8058	176.127	-70.001
-55.835	59.2758	-179.91	-60.14
55.5509	-55.031	-75.794	-67.893
54.536	-57.661	-71.685	-158.45
-56.145	59.7423	177.845	-168.94
53.8894	-56.638	-71.863	-171.06
53.9327	-55.879	-72.945	-175.92
-55.552	58.9647	-179.81	-65.171
55.2564	-56.055	-73.67	-65.409
54.8557	-57.202	-71.17	-58.378

53.9306	-55.815	-73.049	-176.4
53.9255	-56.656	-71.858	-170.75
54.0071	-56.735	-71.885	-169.37
54.273	-57.286	-70.247	-62.046
54.8606	-57.221	-71.166	-58.057
54.8167	-57.657	-70.547	-57.785
55.2448	-55.811	-74.03	-65.892
-55.47	59.0859	-179.94	-66.963
54.3337	-58.212	-69.045	-56.367
-55.754	59.7254	178.196	179.202
54.2862	-58.106	-69.077	-57.275
53.9815	-56.631	-72.043	-170.21
-55.46	59.0957	179.969	-66.314
54.5401	-56.106	-71.88	-64.069
53.7073	-56.381	-72.162	-171.51
54.5147	-55.977	-72.011	-64.641
54.4824	-55.957	-71.997	-64.889

Compound 39



Molecule (-538.2433033 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	2.3424	0	0.00373	0
Conformer.2	2.80821	0.46581	0.00448	0.00074
Conformer.3	4.69095	2.34855	0.00748	0.00374
Conformer.4	5.77111	3.42871	0.0092	0.00546
Conformer.5	6.32459	3.98219	0.01008	0.00635
Conformer.6	7.1506	4.8082	0.0114	0.00766

Conformation Energies	Relative Energies
-538.2435523	0

-538.2433033	0.000249
-538.2416383	0.001914
-538.2383434	0.005209
-538.237021	0.006531
-538.236226	0.007326

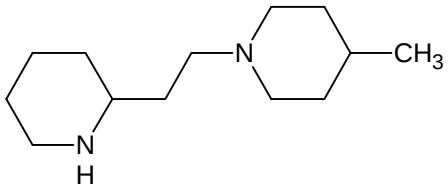
Dih(N2,C8,C12,C11)	Dih(C8,C12,C11,C10)	Dih(C12,C11,C10,N2)
(-22.69) -22.922	(-2.73) -2.5941	(27.24) 27.144
(-22.53) -21.277	(-3.00) -4.3734	(27.55) 28.4017
(-27.05) -27.695	(2.36) 3.36695	(23.10) 22.2074
(-23.07) -22.782	(-2.37) -2.7332	(27.04) 27.2466
(-21.74) -20.746	(-3.84) -4.8928	(28.16) 28.7073
(-27.14) -26.011	(2.37) 0.91394	(23.16) 24.5195

Dih(C10,N2,C7,C4)	Dih(N2,C7,C4,C3)	Dih(C7,C4,C3,C5)	Dih(C4,C3,C5,C1)
(-171.29) -174.33	(55.27) 55.653	(60.33) 59.5241	(174.83) 175.391
(-170.87) -175.11	(167.09) 170.144	(64.30) 61.8658	(175.44) 175.765
(-69.12) -66.019	(-68.90) -71.728	(78.04) 70.3742	(175.91) 174.646
(-171.02) -175.7	(53.82) 54.1128	(64.13) 57.9577	(74.23) 71.6778
(-170.86) -174.66	(166.40) 171.625	(64.69) 63.1423	(74.10) 71.5048
(-71.63) -70.393	(-67.19) -73.257	(84.51) 73.5822	(74.54) 71.1444

Dih(C3,C5,C1,C6)	Dih(C5,C1,C6,C2)	Dih(C1,C6,C2,N1)	Dih(C6,C2,N1,C3)
(-52.89) -52.323	(52.81) 52.2333	(-56.17) -55.992	(62.14) 59.6569
(-52.90) -52.241	(52.71) 52.0933	(-55.98) -55.735	(62.03) 59.7023
(-53.52) -52.166	(52.86) 52.3372	(-55.75) -56.22	(61.66) 59.8591
(53.19) 53.3619	(-53.03) -52.323	(52.87) 53.9435	(-52.16) -55.827
(53.43) 52.9661	(-53.00) -51.807	(52.73) 53.9187	(-52.30) -56.654
(52.37) 52.7102	(-52.48) -51.622	(53.59) 54.4666	(-53.89) -57.58

Dih(C2,N1,C3,C4)	Dih(N1,C3,C4,C7)
(176.27) 178.344	(-179.56) -178.85
(175.86) 177.896	(-175.26) -176.35
(175.55) 177.965	(-161.50) -167.96
(-77.66) -73.01	(-169.45) -176.26
(-77.58) -71.919	(-168.69) -171.28
(-76.68) -72.161	(-148.87) -161.06

Compound 36



Molecule (-616.3181393 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	3.41348	0	0.00544	0
Conformer.2	4.06424	0.65077	0.00648	0.00104
Conformer.3	5.80493	2.39146	0.00925	0.00381
Conformer.4	6.80447	3.391	0.01084	0.0054
Conformer.5	6.97562	3.56214	0.01112	0.00568
Conformer.6	7.56599	4.15252	0.01206	0.00662
Conformer.7	8.16304	4.74956	0.01301	0.00757
Conformer.8	10.1378	6.72432	0.01616	0.01072
Conformer.9	11.9421	8.52866	0.01903	0.01359

Conformation Energies	Relative energy
-616.316168	0.001971
-616.3181393	0
-616.3141656	0.001971
-616.3140521	0.004087
-616.3124246	0.005715

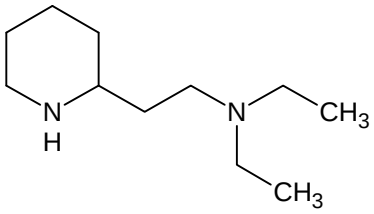
Dih(N2,C13,C12,C11)	Dih(C13,C12,C11,C10)	Dih(C12,C11,C9,C8)
(-55.83) -55.173	(-75.44) -74.461	(-50.27) -50.074
(56.08) 56.2087	(-177.11) -175.88	(52.61) 52.6902
(-55.99) -55.412	(-75.39) -74.408	(-50.12) -50.023
(55.33) 55.3238	(-177.15) -176.35	(53.08) 53.3804
(56.14) 56.2838	(-177.15) -175.87	(52.62) 52.6534
-55.491	-74.218	-50.105
-55.419	-74.678	-49.889
55.3677	-176.34	53.3512
-49.754	-73.012	-51.196
Dih(C11,C9,C8,N2)	Dih(C9,C8,N2,C7)	Dih(C8,N2,C7,C6)
(56.04) 55.3958	(173.09) 176.98	(-164.99) -168.27
(-56.28) -56.279	(-165.63) -171.52	(-67.72) -66.44
(55.78) 55.1804	(174.46) 177.934	(-72.19) -67.274
(-56.17) -55.502	(-161.71) -169.32	(-83.11) -87.677
(-56.30) -56.282	(-165.61) -171.49	(-65.58) -66.122
55.0074	179.101	-67.931
55.5276	177.479	-71.752
-55.56	-169.5	-87.938
48.8798	95.5487	-77.162

Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)
(59.25) 59.3035	(174.97) 175.48	(-52.85) -52.353	(52.73) 52.232
(65.22) 63.2806	(175.61) 175.453	(-52.92) -52.287	(52.69) 52.2302
(78.55) 72.1377	(175.73) 174.551	(-53.48) -52.203	(52.88) 52.3067
(61.15) 59.2208	(174.88) 176.014	(-53.15) -52.823	(52.62) 52.1113
(71.95) 64.4329	(74.49) 71.4254	(52.70) 52.8989	(-52.65) -51.828
67.7243	71.2612	52.5477	-51.49
73.6846	70.6908	52.9179	-51.537

58.2302	72.0052	53.0611	-52.226
62.9125	175.513	-52.277	52.2122

Dih(C3,C2,C1,N1)	Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,C7)
(-56.13) -55.967	(62.18) 59.6341	(176.07) 178.312	(179.40) -179.05
(-55.98) -55.827	(62.12) 59.5634	(175.75) 178.283	(-174.35) -174.97
(-55.78) -56.213	(61.66) 59.9559	(175.71) 178.044	(-161.05) -166.4
(-55.88) -55.471	(62.22) 59.534	(176.07) 178.088	(-179.22) -179.51
(53.23) 53.9941	(-53.30) -56.634	(-76.69) -72.064	(-161.48) -170.01
54.1813	-57.36	-71.309	-166.94
54.2356	-57.46	-71.977	-161.12
54.0524	-56.101	-72.81	-176.07
-55.815	59.5817	178.185	-175.31

Compound 34



Molecule (-539.4008653 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	0.8234	0	0.00131	0
Conformer.2	1.11888	0.29548	0.00178	0.00047
Conformer.3	1.19606	0.37266	0.00191	0.00059
Conformer.4	1.38247	0.55906	0.0022	0.00089
Conformer.5	1.57486	0.75146	0.00251	0.0012
Conformer.6	1.58615	0.76275	0.00253	0.00122
Conformer.7	1.66106	0.83766	0.00265	0.00133
Conformer.8	1.6885	0.8651	0.00269	0.00138
Conformer.9	1.79634	0.97294	0.00286	0.00155

Conformer.10	1.93467	1.11127	0.00308	0.00177
Conformer.11	1.96156	1.13816	0.00313	0.00181
Conformer.12	2.01639	1.19299	0.00321	0.0019
Conformer.13	2.10152	1.27812	0.00335	0.00204
Conformer.14	2.11389	1.29049	0.00337	0.00206
Conformer.15	2.27971	1.45631	0.00363	0.00232
Conformer.16	2.2987	1.4753	0.00366	0.00235
Conformer.17	2.32487	1.50147	0.0037	0.00239
Conformer.18	2.38336	1.55996	0.0038	0.00249
Conformer.19	2.44531	1.62191	0.0039	0.00258
Conformer.20	2.55544	1.73204	0.00407	0.00276
Conformer.21	2.74167	1.91827	0.00437	0.00306
Conformer.22	2.85943	2.03603	0.00456	0.00324
Conformer.23	2.92679	2.10339	0.00466	0.00335
Conformer.24	2.98659	2.16319	0.00476	0.00345
Conformer.25	3.01775	2.19435	0.00481	0.0035
Conformer.26	3.11043	2.28703	0.00496	0.00364
Conformer.27	3.13957	2.31617	0.005	0.00369
Conformer.28	3.20184	2.37844	0.0051	0.00379
Conformer.29	3.22131	2.39791	0.00513	0.00382
Conformer.30	3.34605	2.52265	0.00533	0.00402
Conformer.31	3.35179	2.52839	0.00534	0.00403
Conformer.32	3.36972	2.54632	0.00537	0.00406
Conformer.33	3.42604	2.60264	0.00546	0.00415
Conformer.34	3.46672	2.64332	0.00552	0.00421
Conformer.35	3.56184	2.73844	0.00568	0.00436
Conformer.36	3.56588	2.74248	0.00568	0.00437
Conformer.37	3.6143	2.7909	0.00576	0.00445
Conformer.38	3.63672	2.81332	0.0058	0.00448
Conformer.39	3.64451	2.82111	0.00581	0.0045
Conformer.40	3.7418	2.9184	0.00596	0.00465
Conformer.41	3.74427	2.92087	0.00597	0.00465
Conformer.42	4.10235	3.27895	0.00654	0.00523
Conformer.43	4.16333	3.33993	0.00663	0.00532
Conformer.44	4.18465	3.36125	0.00667	0.00536
Conformer.45	4.24712	3.42372	0.00677	0.00546
Conformer.46	4.26972	3.44632	0.0068	0.00549

Conformer.47	4.27028	3.44688	0.00681	0.00549
Conformer.48	4.27417	3.45077	0.00681	0.0055
Conformer.49	4.2897	3.4663	0.00684	0.00552
Conformer.50	4.31175	3.48835	0.00687	0.00556
Conformer.51	4.31191	3.48851	0.00687	0.00556
Conformer.52	4.3789	3.5555	0.00698	0.00567
Conformer.53	4.40216	3.57877	0.00702	0.0057
Conformer.54	4.42037	3.59697	0.00704	0.00573
Conformer.55	4.46778	3.64438	0.00712	0.00581
Conformer.56	4.47474	3.65134	0.00713	0.00582
Conformer.57	4.48813	3.66473	0.00715	0.00584
Conformer.58	4.48943	3.66603	0.00715	0.00584
Conformer.59	4.53249	3.70909	0.00722	0.00591
Conformer.60	4.57533	3.75194	0.00729	0.00598
Conformer.61	4.64234	3.81894	0.0074	0.00609
Conformer.62	4.81347	3.99007	0.00767	0.00636
Conformer.63	4.8797	4.0563	0.00778	0.00646
Conformer.64	4.88205	4.05865	0.00778	0.00647
Conformer.65	5.12829	4.30489	0.00817	0.00686
Conformer.66	5.14939	4.32599	0.00821	0.00689
Conformer.67	5.17595	4.35255	0.00825	0.00694
Conformer.68	5.18674	4.36334	0.00827	0.00695
Conformer.69	5.21488	4.39148	0.00831	0.007
Conformer.70	5.22341	4.40001	0.00832	0.00701
Conformer.71	5.22803	4.40463	0.00833	0.00702
Conformer.72	5.23938	4.41598	0.00835	0.00704
Conformer.73	5.33488	4.51148	0.0085	0.00719
Conformer.74	5.35197	4.52857	0.00853	0.00722
Conformer.75	5.37665	4.55325	0.00857	0.00726
Conformer.76	5.44681	4.62341	0.00868	0.00737
Conformer.77	5.45991	4.63651	0.0087	0.00739
Conformer.78	5.61662	4.79322	0.00895	0.00764
Conformer.79	5.63964	4.81624	0.00899	0.00768
Conformer.80	5.67479	4.85139	0.00904	0.00773
Conformer.81	5.85446	5.03106	0.00933	0.00802
Conformer.82	5.97154	5.14814	0.00952	0.0082
Conformer.83	6.01401	5.19061	0.00958	0.00827

Conformer.84	6.26953	5.44613	0.00999	0.00868
Conformer.85	6.53511	5.71171	0.01041	0.0091
Conformer.86	6.57409	5.75069	0.01048	0.00916
Conformer.87	6.78006	5.95666	0.0108	0.00949
Conformer.88	6.95352	6.13012	0.01108	0.00977
Conformer.89	7.13254	6.30914	0.01137	0.01005
Conformer.90	7.19312	6.36972	0.01146	0.01015
Conformer.91	7.92847	7.10507	0.01263	0.01132
Conformer.92	8.00235	7.17895	0.01275	0.01144
Conformer.93	8.40951	7.58611	0.0134	0.01209
Conformer.94	8.41133	7.58793	0.0134	0.01209
Conformer.95	8.59317	7.76977	0.01369	0.01238
Conformer.96	8.76756	7.94416	0.01397	0.01266
Conformer.97	9.05239	8.22899	0.01443	0.01311
Conformer.98	9.09644	8.27304	0.0145	0.01318
Conformer.99	9.62184	8.79844	0.01533	0.01402
Conformer.100	9.67585	8.85245	0.01542	0.01411

Conformation Energies	Relative Energy
-539.4021674	0.003011
-539.401499	0.003679
-539.401121	0.004057
-539.4051784	0
-539.4032266	0.001952

Dih(C9,C8,N2,C7)	Dih(C11,C10,N2,C7)	Dih(C8,N2,C7,C6)	Dih(C10,N2,C7,C6)
(79.35) 76.2402	(-151.73) -160.4	(-154.72) -164.41	(78.08) 72.5424
(64.72) 61.6226	(78.68) 73.6641	(61.48) 61.17	(-166.54) -171.7
(67.43) 64.6821	(168.47) 172.001	(62.27) 61.4655	(-164.84) -169.46
(80.48) 77.9064	(-153.41) -161.73	(-156.04) -161.28	(77.41) 75.8269
(-80.12) -77.023	(155.66) 160.075	(163.22) 162.952	(-70.11) -73.866
58.4943	-57.911	62.2655	-64.899
57.3802	-159.21	59.6772	-68.071
77.4328	-159.59	-160.31	76.6781
-66.473	-173.46	-159.66	71.9796

-62.333	-171.83	-59.87	171.465
-59.571	-71.848	-58.691	174.556
-64.593	-172.03	-60.905	170.147
172.514	66.366	-166.48	64.9852
75.3576	63.0432	-168.54	64.8593
-60.119	-71.12	-57.527	175.375
58.0291	-58.499	64.1807	-62.961
159.406	-77.642	-77.559	159.547
159.376	-57.214	67.4866	-60.265
57.8855	-58.197	63.9607	-63.585
56.1073	-160.18	60.8956	-67.321
66.7614	-70.567	-113.26	123.022
-65.814	70.5561	111.64	-124.06
120.551	-167.42	-70.656	164.598
-60.945	167.703	98.8292	-137.46
78.2593	-161.2	-157.36	79.8564
-169.91	127.558	162.733	-72.595
78.2769	-157.92	-154.49	82.3514
75.3351	-62.198	-140.73	97.191
-77.601	158.506	161.426	-75.037
71.0944	59.4508	-175.2	57.3369
171.229	62.0007	-172.12	58.5555
-165.63	116.257	166.758	-68.095
-167.96	122.408	163.444	-71.27
172.985	-135.95	-160.43	76.1258
-65.797	-170.87	-153.84	77.9277
159.057	-78.359	-80.336	157.213
-61.921	-171.79	-59.636	171.792
-59.466	-71.857	-58.595	174.714
-73.185	-60.895	172.489	-60.216
-62.045	-103.27	-165.69	66.3716
63.0163	-72.657	-96.876	141.391
57.8223	-58.668	63.5319	-63.972
61.5225	-168.72	-104.09	131.439
159.101	-57.495	67.0967	-60.99
168.166	-122.87	-163.03	71.6634
56.2932	-160.02	60.7137	-67.421

70.721	172.404	73.8837	-157.16
45.4979	-67.205	63.4863	-160.29
66.5081	65.0841	-96.736	136.231
-64.568	-65.492	-137.05	96.0897
76.971	68.1199	-158.6	74.4177
57.9182	-58.185	64.6856	-62.757
-60.412	-73.165	-60.527	171.801
58.187	-58.189	62.2456	-64.792
57.1541	-159.46	59.7174	-67.908
171.689	61.9124	-170.69	60.3641
72.2091	59.115	-173.62	59.3361
61.846	73.2866	60.3122	-172.57
61.0664	108.16	164.447	-66.688
64.8676	172.001	60.6461	-170.31
119.895	-167.22	-70.477	164.843
-91.93	-58.01	71.2451	-64.793
160.03	-76.515	-73.135	163.398
171.365	62.0038	-171.98	58.967
61.958	-67.671	44.4505	-88.111
-45.628	67.169	-63.029	160.824
77.8315	-158.63	-157.76	79.0368
168.516	-61.343	-132.95	103.516
66.9832	-69.433	-114.98	120.695
-45.024	67.5244	-63.104	160.839
-67.085	-175.31	-160.14	70.7783
74.2303	-62.59	-138.97	100.47
150.703	-60.612	82.579	-49.076
-67.099	43.9099	-160.13	64.8741
-77.936	158.718	159.756	-76.946
-68.781	-62.873	91.4792	-44.861
156.997	-68.169	44.1223	-88.572
-77.655	158.411	153.864	-82.637
-92.463	-159.74	68.5246	-68.621
174.968	-146.22	-156.92	80.1511
66.6698	172.22	157.632	-73.531
68.1699	177.443	163.024	-67.232
-67.785	43.8618	-160.12	63.7355

-60.34	-73.144	-60.518	171.906
104.966	61.6841	-67.014	164.817
-44.907	67.2824	-63.863	160.431
-59.875	168.146	94.9787	-141.32
-168.64	123.976	162.219	-72.346
-68.806	-62.829	91.3845	-44.945
-67.662	43.4298	-159.85	64.5149
151.275	-60.945	82.7363	-48.192
-152.56	61.1561	-84.132	47.5168
61.6871	-61.505	85.4006	-45.802
-67.572	62.3424	-88.256	43.9868
154.661	-60.614	61.5617	-68.161
-158.88	60.7144	-45.898	85.6199
-44.385	67.9772	-63.601	159.881
-46.537	64.7261	-160.38	62.7838
58.7264	-157.12	80.0485	-52.398
-82.255	-66.679	114.365	-32.885

Dih(N2,C7,C6,C5)	Dih(C7,C6,C5,C4)	Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)
(63.49) 52.8728	(70.61) 60.2678	(175.81) 175.616	(-53.50) -52.459
(54.47) 55.0508	(61.57) 59.5939	(175.01) 175.395	(-53.01) -52.336
(52.84) 54.2834	(59.04) 59.5514	(174.87) 175.395	(-52.85) -52.336
(66.00) 60.4525	(164.91) 166.321	(177.26) 178.972	(-52.68) -52.225
(-48.21 -51.821	(-175.35) 178.324	(176.78) 178.028	(-53.23) -52.716
175.265	63.7729	175.398	-52.28
174.522	63.6836	175.4	-52.287
169.537	61.9048	175.829	-52.25
60.5586	166.586	179.013	-52.261
-170.32	174.518	178.066	-52.365
-170.92	174.432	178.062	-52.367
-53.901	177.402	177.9	-52.753
63.1112	167.663	179.254	-52.254
63.9882	167.659	179.325	-52.233
-169.13	172.651	178.088	-52.897
-176.35	170.404	178.127	-52.913
-170.71	172.622	178.118	-52.901
-175.52	170.545	178.106	-52.912

-177	173.694	178.074	-52.384
-177.69	173.548	178.124	-52.371
-176.62	174.598	177.974	-52.421
174.27	62.9739	175.806	-52.229
-173.73	174.162	178.044	-52.371
56.1105	61.8638	175.724	-52.555
65.2218	166.643	75.7703	52.727
-57.432	175.877	177.902	-52.8
-174.83	171.848	178.539	-52.896
57.4661	164.39	178.874	-52.231
-69.271	72.7975	174.467	-52.165
178.438	169.364	178.574	-52.906
177.956	169.415	178.564	-52.907
-171.45	172.329	178.093	-52.903
176.435	63.0213	175.726	-52.241
66.443	166.805	179.231	-52.197
65.4861	166.91	76.1131	52.7834
-173.83	175.236	74.368	51.5498
-170.13	175.522	74.408	51.6016
-170.49	175.357	74.4375	51.6242
-71.807	69.5901	174.994	-52.282
169.034	61.6597	175.744	-52.24
-60.783	168.982	177.908	-52.862
-176.45	174.351	74.3636	51.7682
-174.41	171.825	178.221	-52.907
-175.05	174.441	74.4388	51.7709
-176.25	171.46	178.547	-52.892
-177.65	174.469	74.2805	51.7477
66.9009	166.585	76.5263	52.8562
56.3902	59.5332	175.357	-52.305
-55.304	175.437	177.957	-52.804
58.6138	164.481	178.947	-52.225
67.3584	166.272	76.4718	52.8819
-176.27	171.683	74.3294	52.3966
-63.541	168.947	178.066	-52.386
175.972	64.8933	71.3589	52.889
175.06	64.8919	71.4571	52.8346

178.507	175.839	74.2783	51.5725
178.997	175.956	74.2677	51.5589
53.9775	58.1165	71.6347	53.3299
-179.98	64.3404	175.632	-52.264
53.2445	58.24	71.6809	53.2976
-173.57	175.147	74.3254	51.5945
169.924	62.1997	175.599	-52.289
-52.085	179.111	74.4373	51.5519
176.88	170.339	74.2266	52.5601
65.8877	61.0489	176.1	-52.952
-56.415	176.568	177.92	-52.785
173.018	63.975	71.5357	52.9026
65.7614	164.311	75.9408	53.0424
-175.89	171.314	74.4003	52.4183
-172.2	171.771	178.123	-52.902
169.475	62.7072	71.6181	52.9612
64.3821	162.099	76.1075	53.2008
-66.072	176.691	178.281	-52.926
66.4609	167.233	179.325	-52.248
-70.744	73.1459	69.9169	53.3607
-172.38	174.792	178.075	-52.388
66.3489	60.9015	176.107	-52.951
-67.171	169.921	74.0258	52.573
176.751	168.826	178.144	-52.933
67.8542	163.584	76.1545	52.8398
-69.836	73.5721	70.3308	53.0942
102.475	68.3787	176.039	-52.798
-177.01	171.203	178.549	-52.886
-63.396	169.546	74.0836	52.6207
-170.8	172.505	74.4089	52.2984
-171.65	174.781	74.6123	51.715
51.5957	58.8528	71.737	53.268
-66.873	169.118	74.0091	52.6503
-171.95	175.501	74.4237	51.6658
-177.68	176.072	74.3384	51.5808
-66.97	179.082	74.5821	51.4272
65.9917	60.1429	72.0007	52.8694

-66.994	179.338	74.5767	51.3995
65.0827	60.0791	71.9836	52.8801
91.0815	65.858	72.2591	52.6777
-67.376	179.321	74.5779	51.3931
-65.805	169.712	74.0242	52.5817
-95.332	171.059	177.716	-53.005
-73.779	112.008	178.043	-53.866
-70.1	171.564	177.674	-53.045

Dih(C4,C3,C2,C1)		Dih(C3,C2,C1,N1)		Dih(C2,C1,N1,C5)	
(52.67)	52.1754	(-55.87)	-55.897	(62.21)	59.701
(52.73)	52.2404	(-56.04)	-55.972	(62.13)	59.6271
(52.75)	52.2418	(-56.12)	-55.971	(62.15)	59.6234
(52.31)	50.8054	(-55.92)	-54.752	(62.20)	61.0365
(53.21)	52.2991	(-56.54)	-55.844	(61.29)	59.3686
	52.2244		-55.837		59.5959
	52.2298		-55.829		59.5726
	52.0838		-55.707		59.6881
	50.8935		-54.806		60.9505
	51.7712		-55.442		59.2599
	51.7687		-55.44		59.2649
	52.36		-55.835		59.257
	50.9423		-54.824		60.8712
	50.8979		-54.8		60.915
	52.3681		-55.559		58.9734
	52.2548		-55.456		59.1303
	52.3859		-55.562		58.9378
	52.2549		-55.448		59.1191
	51.7816		-55.395		59.2637
	51.7529		-55.392		59.3034
	51.8959		-55.455		59.0686
	52.058		-55.696		59.7527
	51.7774		-55.442		59.2452
	52.07		-55.814		59.9001
	-53.304		55.2415		-55.943
	52.3841		-55.867		59.2614
	52.2665		-55.435		59.0767

50.629	-54.623	61.2568
52.3067	-56.229	59.958
52.1404	-55.342	59.2538
52.1468	-55.345	59.2428
52.3754	-55.557	58.958
52.1522	-55.752	59.641
50.7268	-54.589	61.0223
-53.447	55.2604	-55.741
-51.724	54.8962	-57.268
-51.777	54.8585	-57.163
-51.81	54.8672	-57.13
52.3287	-56.119	59.7753
52.1089	-55.739	59.6741
51.9535	-55.604	59.8725
-51.837	54.761	-57.115
52.3372	-55.508	58.9931
-51.88	54.7879	-57.071
52.2378	-55.41	59.1079
-51.776	54.7177	-57.144
-53.66	55.3364	-55.48
52.229	-55.987	59.6732
52.2713	-55.814	59.4322
50.652	-54.606	61.1802
-53.664	55.3205	-55.465
-51.771	54.1587	-57.304
51.3406	-55.351	60.022
-51.805	53.9971	-56.671
-51.818	54.0402	-56.681
-51.479	54.7939	-57.712
-51.456	54.7853	-57.74
-52.279	53.9342	-55.87
52.1537	-55.762	59.6764
-52.282	53.9585	-55.885
-51.746	54.8645	-57.215
52.2194	-55.801	59.5356
-51.226	54.375	-58.306
-51.763	54.1918	-57.434

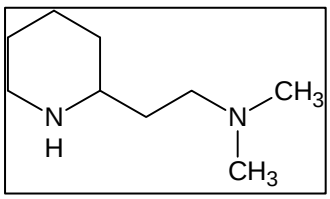
52.0418	-55.389	59.6254
52.3588	-55.83	59.2714
-51.773	53.9394	-56.714
-53.64	55.2177	-55.38
-51.868	54.3285	-57.288
52.3275	-55.523	59.0246
-51.841	53.9205	-56.582
-53.963	55.2655	-54.98
52.0227	-55.327	59.4854
50.8738	-54.747	60.9181
-51.493	53.8488	-57.184
51.8353	-55.408	59.1748
52.0504	-55.387	59.6015
-52.452	54.5406	-56.077
52.2187	-55.438	59.2019
-53.77	55.6554	-55.695
-51.485	54.0536	-57.362
51.9176	-55.366	59.9241
52.2227	-55.412	59.1378
-52.526	54.4977	-55.925
-51.794	54.2647	-57.269
-51.932	54.9253	-57.051
-52.276	54.0224	-56.031
-52.52	54.5001	-55.938
-51.756	54.7721	-57.203
-51.546	54.8236	-57.609
-51.629	54.9227	-57.524
-52.114	54.1622	-56.378
-51.605	54.9196	-57.568
-52.113	54.1563	-56.357
-52.026	54.2563	-56.985
-51.615	54.9234	-57.551
-52.452	54.5131	-56.055
52.2676	-55.506	59.1944
51.7847	-54.759	59.7188
52.1348	-55.408	59.4565

Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,C7)
(175.99) 178.235	(-169.72) -178.23
(176.21) 178.359	(-178.45) -178.78
(176.18) 178.365	(179.17) -178.82
(176.59) 175.857	(-74.40) -72.451
(178.85) 179.921	(-54.65) -59.779
178.324	-174.54
178.361	-174.62
177.903	-176.31
176.085	-72.126
178.968	-63.174
178.967	-63.27
-179.83	-60.733
176.134	-70.858
175.999	-70.848
-179.79	-65.417
-179.98	-67.842
-179.78	-65.398
-179.97	-67.703
179.022	-64.035
178.942	-64.178
179.283	-63.029
177.828	-175.27
178.99	-63.533
178.02	-176.89
-73.73	-66.562
-179.72	-62.314
179.87	-66.138
175.5	-74.669
178.208	-165.78
179.65	-68.811
179.667	-68.756
-179.77	-65.732
177.885	-175.1
175.631	-71.864
-74.157	-66.119
-71.139	-58.581

-71.232	-58.297
-71.292	-58.445
177.691	-168.62
177.926	-176.54
179.587	-69.931
-71.185	-59.521
-179.9	-66.224
-71.304	-59.385
179.82	-66.557
-71.071	-59.442
-74.753	-66.208
178.301	-178.84
-179.93	-62.91
175.537	-74.479
-74.731	-66.544
-70.092	-62.728
178.403	-69.561
-71.971	-169.62
-72.01	-169.59
-70.442	-58.011
-70.39	-57.906
-72.964	-176.12
177.95	-173.88
-72.965	-175.99
-71.135	-58.697
178.2	-175.98
-69.011	-55.651
-69.945	-64.007
178.056	-177.91
-179.77	-61.623
-71.792	-170.48
-74.508	-68.731
-70.316	-62.94
-179.88	-66.342
-72.017	-171.65
-75.139	-70.952
179.637	-61.907

175.983	-71.32
-71.597	-161.87
179.111	-62.854
178.094	-178.04
-71.912	-64.333
179.99	-69.512
-74.65	-69.358
-71.783	-161.35
178.1	-170.81
179.78	-66.829
-72.071	-64.699
-70.25	-61.822
-71.537	-58.9
-72.881	-175.54
-72.029	-65.119
-71.128	-58.329
-70.629	-57.727
-70.847	-55.075
-72.591	-174.31
-70.793	-54.871
-72.555	-174.41
-71.851	-169.15
-70.82	-54.888
-71.902	-64.547
-179.61	-67.588
178.183	-127.67
-179.95	-67.368

Compound 35



Molecule (-461.3333405 au)	E gas(kcal/mol)	Rel. E gas(kcal/mol)	E gas(au)	Rel. E gas(au)
Conformer.1	4.81494	0	0.00767	0
Conformer.2	5.26518	0.45024	0.00839	0.00072
Conformer.3	6.10891	1.29397	0.00974	0.00206
Conformer.4	6.71003	1.89509	0.01069	0.00302
Conformer.5	7.30466	2.48972	0.01164	0.00397
Conformer.6	7.98705	3.17211	0.01273	0.00506
Conformer.7	8.21911	3.40417	0.0131	0.00542
Conformer.8	8.73037	3.91543	0.01391	0.00624
Conformer.9	8.81208	3.99714	0.01404	0.00637
Conformer.10	9.61841	4.80347	0.01533	0.00765
Conformer.11	9.6368	4.82186	0.01536	0.00768
Conformer.12	9.75446	4.93952	0.01554	0.00787
Conformer.13	10.4133	5.59833	0.01659	0.00892
Conformer.14	11.6272	6.81226	0.01853	0.01086
Conformer.15	12.9235	8.10858	0.02059	0.01292
Conformer.16	13.0701	8.25513	0.02083	0.01316

Conformation Energy	Relative Energies
-461.3343895	0
-461.334119	0.00027
-461.3333405	0.001049
-461.332381	0.002008
-461.332424	0.001965

Dih(C9,N2,C7,C6)	Dih(C8,N2,C7,C6)	Dih(N2,C7,C6,C5)	Dih(C7,C6,C5,C4)
(-167.20) -170.06	(66.99) 67.769	(53.31) 54.3403	(59.54) 59.5001
(-167.39) -171.27	(66.78) 66.4477	(163.69) 168.394	(63.75) 61.6084

(-71.63) -69.267	(162.42) 168.533	(-178.81) 179.778	(66.95) 64.1722
(65.29) 61.4068	(-67.58) -65.551	(173.28) 174.599	(64.89) 63.329
(-69.97) -66.703	(164.43) 170.921	(-66.99) -69.761	(79.11) 71.5422
-170.35	67.2185	53.8633	58.2493
-171.53	66.2372	52.8079	57.9918
-66.978	170.852	-177.07	67.4955
-170.76	66.7492	169.667	62.6939
44.5798	-86.545	66.1337	58.9731
61.4044	-65.42	174.99	64.4467
-71.197	166.875	-71.027	74.5133
85.9878	-45.022	-65.136	178.517
-170.29	67.6626	-101.47	173.196
44.009	-86.86	65.3648	58.0691
-64.558	172.309	101.448	68.8574

Dih(C6,C5,C4,C3)	Dih(C5,C4,C3,C2)	Dih(C4,C3,C2,C1)	Dih(C3,C2,C1,N1)
(174.89) 175.405	(-52.78) -52.341	(52.75)52.2341	(-56.14) -55.98
(175.40) 175.798	(-52.90) -52.254	(52.73) 52.1011	(-55.99) -55.723
(175.44) 175.661	(-53.00) -52.265	(52.70) 52.153	(-55.95)-55.757
(175.55) 175.449	(-52.94)-52.289	(52.76) 52.2318	(-56.01) -55.827
(175.79) 174.646	(-53.50) -52.219	(52.88) 52.3109	(-55.76) -56.187
71.8203	53.6032	-52.402	53.6798
71.7333	53.3197	-52.323	53.9699
71.3017	52.5527	-51.509	54.1835
71.6295	52.9571	-51.85	53.9329
175.905	-52.777	52.1311	-55.507
71.4528	52.8928	-51.836	54.0062
70.9486	52.7306	-51.555	54.3924
178.258	-52.912	52.0969	-55.373
74.0263	52.0571	-52.021	54.6468
71.9801	53.0936	-52.228	54.0283
72.2423	51.7887	-51.51	54.6887

Dih(C2,C1,N1,C5)	Dih(C1,N1,C5,C6)	Dih(N1,C5,C6,C7)
(62.12) 59.6477	(176.22) 178.36	(179.66) -178.89
(62.01) 59.67	(175.94) 177.922	(-175.83) -176.59

(62.13) 59.6738	(175.79) 177.926	(-172.78) -174.03
(62.08)59.5618	(175.84) 178.288	(-174.68) -174.93
(61.63) 59.9027	(175.71) 178.004	(-160.48) -166.92
-55.907	-72.611	-176.29
-55.844	-73.027	-176.22
-57.329	-71.357	-167.14
-56.588	-72.045	-171.66
59.5244	178.147	-179.73
-56.633	-72.091	-169.99
-57.587	-71.965	-160.27
59.3741	179.729	-59.947
-56.693	-71.322	-60.956
-56.079	-72.828	-176.22
-57.7	-71.158	-166.09